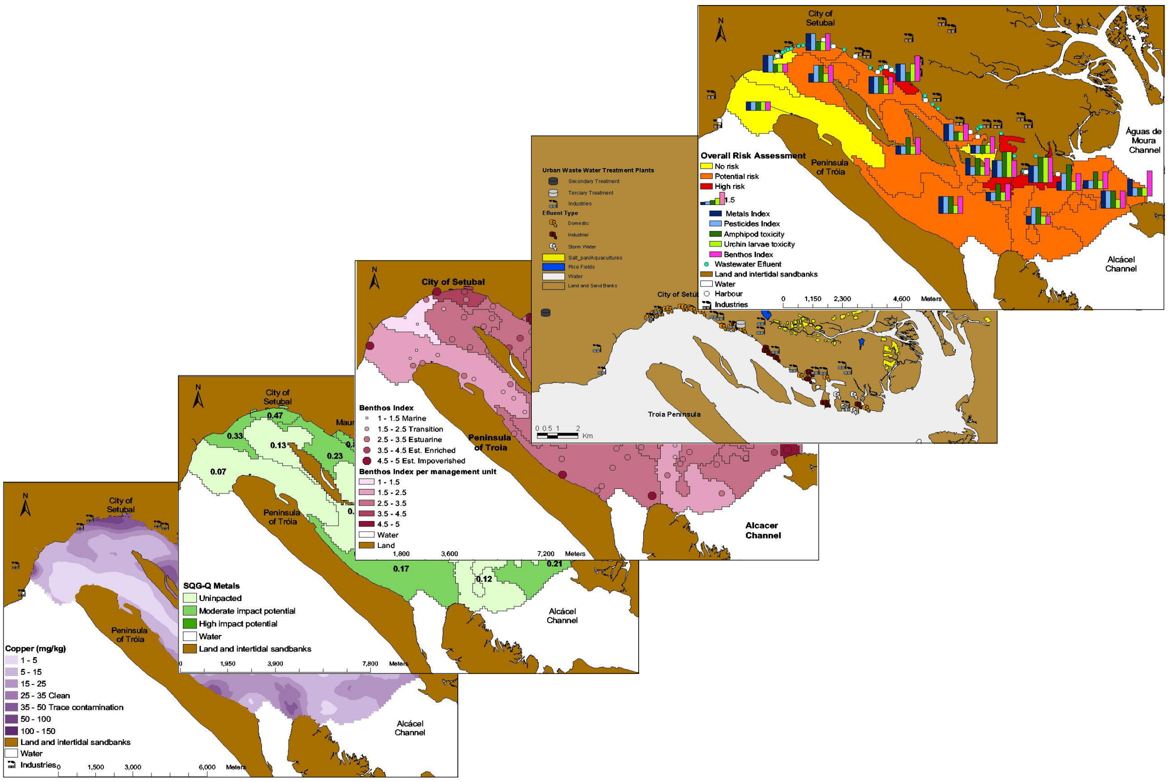
SANDRA SOFIA FERREIRA DA SILVA CAEIRO

ENVIRONMENTAL DATA MANAGEMENT IN THE SADO ESTUARY:

WEIGHT OF EVIDENCE TO ASSESS SEDIMENT QUALITY



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ENVIRONMENTAL DATA MANAGEMENT IN THE SADO ESTUARY: WEIGHT OF EVIDENCE TO ASSESS SEDIMENT QUALITY

Thesis submitted to the Universidade Nova de Lisboa, Faculdade de Ciências e Tecnologia for the degree of Doctor of Philosophy in Environmental Engineering

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Author's declaration

The author states that she afforded a major contribution to the conceptual design and technical execution of the work, interpretation of the results and manuscript preparation of the published articles included in this dissertation, according to the *nº 2 of art. 8º do Decreto –Lei 388/70.*

Sandra Sofia Ferreira da Silva Caeiro

He uses statistics as a drunken man uses lamp-posts... for support rather than illumination.

Andrew Lang (1844-1912) poet and novelist.

To my life companion

… O! learn to read what silent love hath writ:
To hear with eyes belongs to love's fine wit.

William Shakespeare (1564–1616)
Sonnet XXIII *As an unperfect actor on the stage*

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ABSTRACT

Estuaries are perhaps the most threatened environments in the coastal fringe; the coincidence of high natural value and attractiveness for human use has led to conflicts between conservation and development. These conflicts occur in the Sado Estuary since its location is near the industrialised zone of Peninsula of Setúbal and at the same time, a great part of the Estuary is classified as a Natural Reserve due to its high biodiversity. These facts led us to the need of implementing a model of environmental management and quality assessment, based on methodologies that enable the assessment of the Sado Estuary quality and evaluation of the human pressures in the estuary. These methodologies are based on indicators that can better depict the state of the environment and not necessarily all that could be measured or analysed. Sediments have always been considered as an important temporary source of some compounds or a sink for other type of materials or an interface where a great diversity of biogeochemical transformations occur. For all this they are of great importance in the formulation of coastal management system. Many authors have been using sediments to monitor aquatic contamination, showing great advantages when compared to the sampling of the traditional water column.

The main objective of this thesis was to develop an estuary environmental management framework applied to Sado Estuary using the DPSIR Model (EMMSado), including data collection, data processing and data analysis. The support infrastructure of EMMSado were a set of spatially contiguous and homogeneous regions of sediment structure (management units). The environmental quality of the estuary was assessed through the sediment quality assessment and integrated in a preliminary stage with the human pressure for development. Besides the earlier explained advantages, studying the quality of the estuary mainly based on the indicators and indexes of the sediment compartment also turns this methodology easier, faster and human and financial resource saving. These are essential factors to an efficient environmental management of coastal areas. Data management, visualization, processing and analysis was obtained through the combined use of indicators and indices, sampling optimization techniques, Geographical Information Systems, remote sensing, statistics for spatial data, Global Positioning Systems and best expert judgments.

As a global conclusion, from the nineteen management units delineated and analyzed three showed no ecological risk (18.5 % of the study area). The areas of more concern (5.6 % of the study area) are located in the North Channel and are under strong human pressure mainly due

to industrial activities. These areas have also low hydrodynamics and are, thus associated with high levels of deposition. In particular the areas near Lisnave and Eurominas industries can also accumulate the contamination coming from Águas de Moura Channel, since particles coming from that channel can settle down in that area due to residual flow. In these areas the contaminants of concern, from those analyzed, are the heavy metals and metalloids (Cd, Cu, Zn and As exceeded the PEL guidelines) and the pesticides BHC isomers, heptachlor, isodrin, DDT and metabolits, endosulfan and endrin. In the remain management units (76 % of the study area) there is a moderate impact potential of occurrence of adverse ecological effects and in some of these areas no stress agents could be identified. This emphasizes the need for further research, since unmeasured chemicals may be causing or contributing to these adverse effects. Special attention must be taken to the units with moderate impact potential of occurrence of adverse ecological effects, located inside the natural reserve. Non-point source pollution coming from agriculture and aquaculture activities also seem to contribute with important pollution load into the estuary entering from Águas de Moura Channel. This pressure is expressed in a moderate impact potential for ecological risk existent in the areas near the entrance of this Channel. Pressures may also came from Alcácer Channel although they were not quantified in this study.

The management framework presented here, including all the methodological tools may be applied and tested in other estuarine ecosystems, which will also allow a comparison between estuarine ecosystems in other parts of the globe.

RESUMO

As zonas costeiras e, em particular, os estuários, como é o caso de *Estuário do Sado*, devido à sua localização em uma transição entre o meio terrestre e meio marinho, estão sujeitas a inúmeros problemas de contaminação e, ao mesmo tempo, encontram-se dependentes de conflitos de difícil gestão ambiental. Sendo áreas de especial susceptibilidade e importância como ecossistemas muito produtivos, torna-se necessário implementar modelos de avaliação e gestão, que passem pela elaboração de metodologias que não só qualifiquem como quantifiquem as principais fontes e a qualidade do ecossistema procedente dos seus diversos compartimentos: coluna de água, sedimento e biota. Estas metodologias de gestão ambiental podem basear-se na utilização de indicadores e índices, isto é, podem ter acesso à utilização de variáveis ambientais que melhor espelhem os objectivos em causa, e não à totalidade das possibilidades que possam ser medidas e/ou analisadas. Diversos autores têm usado os sedimentos para monitorizar a contaminação de sistemas aquáticos, demonstrando vantagens evidentes em relação à utilização de amostras de água, uma vez que as concentrações de contaminantes nos sedimentos são, em geral, significativamente superiores às concentrações na coluna de água.

O objectivo geral deste trabalho foi implementar um modelo de gestão de informação ambiental para o *Estuário do Sado*, utilizando o modelo conceptual de indicadores *DPSIR (Actividades humanas, Pressão, Estado, Impacte e Resposta)*, que inclui a recolha, tratamento e análise da informação e ainda com base num sistema de informação geográfica. O estudo da qualidade e propriedades do *Estuário* é efectuado através da avaliação da qualidade sedimentar e integração, numa fase preliminar, com as pressões humanas associadas ao desenvolvimento urbano e industrial. Além das vantagens, já referidas anteriormente, sobre a utilização do compartimento sedimentar na avaliação da qualidade do ecossistema, o recurso a indicadores e índices focalizados no compartimento sedimentar, converte esta metodologia em uma forma menos dispendiosa em recursos humanos e financeiros, transforma-a em meios mais rápidos e dirigidos, conduzindo a maior eficiência nos processos de gestão ambiental. A gestão da informação, visualização, processamento e análise foram obtidas através do aproveitamento simultâneo de indicadores e índices ambientais, técnicas de optimização de amostragem, sistemas de informação geográfica, análise estatística espacial, detecção remota, receptores GPS (Sistemas de Posicionamento Global) por navegação por satélite e avaliação pericial. Pretendeu-se, deste modo, delimitar e, posteriormente, caracterizar unidades de gestão ambiental (áreas homogéneas de estrutura sedimentar e contíguas espacialmente) a

partir das quais se poderão aplicar instrumentos para uma gestão sustentável das actividades humanas no *Estuário*, tendo em conta factores económicos, sociais e ambientais.

Como conclusão global, das 19 unidades de gestão delineadas e analisadas, três não apresentam qualquer risco ecológico (o que corresponde a 18,5 % da área de estudo). As áreas de maior alerta, onde será imprescindível desenvolver processos de vigilância e medidas de gestão (5,6 % da área de estudo), estão localizadas no *Canal Norte* e sofrem uma elevada pressão das actividades humanas. Estas áreas apresentam um importante baixo hidrodinamismo, pelo que estão associadas, naturalmente, a elevados níveis de deposição sedimentar. Em particular, é de relevar as áreas adjacente às indústrias *Lisnave* e *Eurominas* que têm, além disso, a possibilidade de acumular também contaminação originária do *Canal de Águas de Moura*, uma vez que as partículas que provêm deste canal podem depositar-se nessa área, devido a correntes residuais. Nessas áreas, portanto, os poluentes mais inquietantes, provenientes da lista dos parâmetros analisados, são principalmente os seguintes: metais pesados e metalóides (o cádmio, o cobre, o zinco e o arsénio apresentaram valores superiores aos valores guia indicativos de efeitos tóxicos) e os pesticidas organoclorados BHC e isómeros, heptacloro, isodrina, DDT e metabólitos, endosulfão e endrina. Nas restantes unidades homogéneas (correspondentes a 76 % da área de estudo) existem sinais de efeitos biológicos adversos e, em algumas dessas áreas, ainda não foi possível delimitar nem identificar um agente que possa vir a originar aqueles prejudiciais danos. Estas circunstâncias dão ênfase à urgência imperativa de ampliação em maior número de investigações deste tipo, dado que contaminantes não medidos nem avaliados podem estar a ocasionar ou a contribuir para a propagação de consequências nefastas. Poluição difusa resultante de actividades agrícolas e de aquacultura parece apontar similarmente para procedências importantes de cargas de poluição no *Estuário* descendente do *Canal de Águas de Moura*. Esta pressão é expressa como um potencial de risco ecológico existente nas áreas localizadas à entrada daquele canal. Acrescente-se ainda a agravante de algumas daquelas unidades estarem incluídas, em parte ou na sua totalidade, na área protegida da *Reserva Natural do Estuário do Sado*. Do *Canal de Alcácer* podem similarmente surgir outros modos de pressões diversas que não foram, no entanto, ainda quantificados neste estudo.

O modelo de gestão, apresentado neste trabalho, com a inserção de todos os instrumentos metodológicos, poderá ser aferido e aplicado a outros ecossistemas estuarinos, actuação que permitirá, igualmente, a análise comparativa ou contrastiva entre diversos estuários, em qualquer parte do mundo.

ABREVIATIONS

APSS – Administration Port of Setúbal and Sesimbra

BI_{bio} – Benthic Biotope Index

BHC – Hexachlorocyclohexane or Benzene Hexanocloride

BOD – Biological Oxygen Demand

BPJ – Best Professional Judjment

COD – Chemical Oxygen Demand

CZM – Coastal Zone Management

DC – Degree of Contamination Index

DPSIR – *Driving Forces*, *Pressure*, *State* and *Impact* indicators framework

Eh – Redox Potential

EMMSado – Environmental Information Management for Sado Estuary, through the sediment quality assessment

EU – European Union

FA – Factor Analysis

FF – Fine Fraction

FOG – Fat, Oil and Grease

GIS – Geographic Information System

GPS – Global Positioning System

HO – High Organic load management unit

I – Index of metals for Ratio-to-Reference

ICP-AES – Inductively Coupled Plasma Atomic Emission Spectroscopy

ICZM – Integrated Coastal Zone Management

LO – Low Organic load management type

LOE – Line of Evidence

MHO – Medium High Organic load management unit

MO – Medium Organic load management unit

MPI – Metal Pollution Index

MSPI – Marine Sediment Pollution index

N – Nitrogen

NI – Index of metals for new Maximum RTR

Nut. – Nutrients

OF – Objective Function

P – Phosphorus

PAH – Polyaromatic Hydrocarbons

PC – Principal Component

PCA – Principal Component Analysis

PCB – Polychlorinated Biphenyls

PEL – Probable Effect Level

PIN – New Pollution Index

PLI – Pollution Load Index

PSR – *Pressure*, *State*, *Response* indicator Framework

RNES – Natural Reserve of Sado Estuary

RTR – Ratio-to Ratio approach of Sediment Quality Triad

SA – Simulated Annealing

SDA –Stepwise Regression Discriminant Analysis

SQG – Sediment Quality Guideline

SQG-Q – Sediment Quality Guideline Quotient

SQT – Sediment Quality Triad

SQV – Sediment Quality Values

SS – Suspended Solids (total)

TBT – Tributyltin

TEL – Threshold Effect Level

TOM – Total Organic Matter

WOE – Weigh of Evidence

WWTP – Waste Water Treatment Plant

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PART I

GENERAL INTRODUCTION

CHAPTER 1 – INTRODUCTION

GENERAL INTRODUCTION

1.1 COASTAL ZONE MANAGEMENT: THE IMPORTANCE OF THE DATA

Coastal zone management (CZM), also referred as Integrated Coastal Zone Management (ICZM), is an issue that has been largely discussed during the last decades. There are many ways in which the CZM process can be summarized, although as a general definition, CZM can represents a dynamic process which develops and implements a co-ordinated strategy to allocate resources to achieve the conservation and sustainable multiple use of coastal zone (French, 1997).

Coastal management has become the framework of choice in the major international pronouncements and agreements emanating from the United Nations Conference on Environment and Development (UNCED), held in Rio de Janeiro in June 1992 (Chapter 17 of Agenda 21) and underlies the Law of the Sea Convention which came into force in 1994 (Sherman and Duda, 1999). Also the Global Program of Action on Protection of the Marine Environment from Land-Based Activities has been adopted, the implementation of the Conventions on Biological Diversity and on Climate Change are proceeding successfully (Cicin-Sain and Knecht, 1998).

Numerous case studies of CZM practices have been applied in developed and developing countries. Clark (1996), French (1997), Cicin-Sain and Knecht (1998) and Salomons *et al.,* (1999) presented, discussed and compared some of them.

Nevertheless coastal areas continue to experience intense and continuous environmental pressures from a range of driving forces that have been increasing in their intensity over many decades (Turner and Salomons, 1999; Kay and Alder, 2000). Little progress has been made in sustained global actions to reverse their degraded state (Sherman and Duda, 1999). Estuaries, as transitional river-marine environments, continue to be widely recognized as one of the most threatened components of the coastal environment, primarily because they are threatened from both land and sea based impacts (Cooper, 1994).

Coastal use is always associated with conflicts, exemplifying the need for management to address and mitigate the negative consequences of such conflicts and to safeguard coastal values (Moriki *et al.,* 1996). Integrated planning for coastal areas, including land use, resources and pollution management, is needed to solve conflicts that occur frequently among residential, tourist, commercial, industrial, transportation, recreational, and agricultural activities competing within limited space. Coastal zone management role is to sort out the uses and recommend the optimal land use mix in other to advise the decision-makers and managers (Clark, 1996).

Governments are now committed to the policy goal of sustainable development. But the fulfilment of the sub-goal of sustainable utilization of coastal resources via integrated management is likely to prove to be an especially difficult task (Turner and Salomons, 1999). In may ways coastal zones typify the problems and policy challenges presented by the process of Global Environmental Change. These zones are under increasing pressure and are exhibiting unacceptable environmental state changes as a consequence of population growth, urbanization, tourism and other multiple and often conflicting resources usage trends. The mitigation of the resource conflict problems and the practical adaptation of the sustainable economic development policy objective requires innovative policy responses. It should be a process which enables policy makers to strike a socially acceptable balance between conflicting stakeholder resource demands as they manifest themselves in different economic, socio-political, institutional, cultural and environmental contexts (Turner and Bower, 1999). The coast is then a place where the issues of economic development and environmental management, and their interactions with social and cultural values are brought into a sharp relief (Kay and Alder, 2000) and that the costal zone management effectiveness is not an easy task (Cicin-Sain and Knecht, 1998) .

The coastal zones should be analysed in terms of two systems that should interact for a correct management of these resources (Van Der Weide and Vrees, 1999):

i) The natural system which provides space, substratum, renewable and non-renewable resources and which regulates physical, biological and chemical processes in the coastal zone. In economic terms the value of this system if often categorized as natural capital.
ii) The socio-economic system, the individuals, the public and private bodies who use the natural resource system for subsistence, economic and social activities. The importance of this system is expressed in economic terms as the human capital, which includes the people, its social infrastructure and the physical infrastructure.

In addition coastal management does not have to be applied to a country's entire coastal zone simultaneously. It can be implemented first where it is needed most – in those areas having urgent problems and needs (Cicin-Sain and Knecht, 1998).

CZM usually includes four stages (Clark, 1996):

1. Policy formulation - creation of a policy framework to establish goals and to authorize and guide the CZM;
2. Strategic planning - process that explores options and develops an optimum strategy for a management program;
3. Program development - starts after the policy makers accept the strategic planning; a detail master plan is created;
4. Implementation - starts once a master plan is approved and a budget and staff authorized.

Strategic planning is the key step in the process of organizing CZM and where the methods are determined. In this phase scientific information with a strong basis is needed to conduct coastal management, including both the natural and the social sciences (Cicin-Sain and Knecht, 1998). In fact one of the major objectives of coastal zone management is to identify the sources of adverse impacts including a vital first step to determine the present condition of the environment (Cooper, 1994). Without the steps of collecting, gathering, management and assessment of data, difficulties arise in implementing partnership and public participation for policy decision and management plan implementation.

1.2 DATA MANAGEMENT: INDICATORS FRAMEWORKS

The coastal and adjacent ocean constitutes a complex and dynamic environment in which a number of physical, biological, geological and chemical processes take place. For that reason different types of information are needed. In carrying out their duties environmental managers and natural resource planners are often faced with a vast array of scientific information. This information is often highly technical and although it is often interdisciplinary it is seldom adequately integrated (Cooper, 1994). Often the collection of multidisciplinary information is ineffective and, even when adequate data is available, ineffectual transfer of information from scientist to end-user can occur.

There seems to be a gap between experimental work and decision-making, mainly because of the incompatibility of methods for the policy interpretation of scientific analysis. Environmental-ecological aspects appear only theoretically in the actual decision-making process; huge data bases, originated from physical and chemical monitoring of the marine environment, remain unexplored, restricted to academic purpose only (Moriki e*t al.,* 1996). It is important for managers to understand the nature of changes of the marine system even if they are not specialists in all the fields. In addition, there is an increasing involvement by environmental lawyers, environmental economists and numerical modellers, many of whom are unlike to be specialists in marine science, or even to have a science background, and thus they may be unaware of the interlinking and complexity of the marine system. This difficulty may be compounded by an increasing trend to bring in business managers to handle environmental organizations (Elliott, 2002).

This may result in either poor or non-reproductive data collection procedures or sub-optimal utilization of information, which ultimately impact on the quality of coastal zone management decisions (Cooper, 1994).

There is the need to demonstrate the bottom-up processes, for example the manner in which natural changes in the physical system create the conditions for biota colonization and the way in which Man influences those changes. Similarly, there is then the need to show the top-down responses in which the higher marine trophic levels are affected by changes in the lower components. Following all this, there is the need to link science to the causes of change and to the social, economic and legal responses by Man to the change (Elliott, 2002).

Coastal management requires effective decision in a reasonable time-scale. Therefore holistic approaches for data management should be based on realistic methods rather than complicated ones, with high level of detail and time-consuming techniques.

In the content of those stressor-response relationships, it is impossible to completely characterize all the variables, so a selected set of measurements should be made to reflect the most critical components. Such measurements, or indicators, should estimate trend, stressor source and magnitude of effects and lead to thresholds for management or restoration action (Fisher *et al*., 2001).

An indicator is a sign that relays a complex message, potentially from numerous sources, in a simplified and useful manner. The primary uses of an indicator are to characterize current status and to track or predict significant change (Jackson *et al.,* 2000) (see Annex I – indicators concepts). The use of indicators and indices for the evaluation and assessment of the environmental status of different ecosystems is becoming a widespread procedure to analyse the various and often complex components of a system like the marine environments (Casazza *et al.,* 2002).

To assure that indicators serve the purpose for which they are intended and control the way they are specifically selected and developed, it is important to organize them in a consistent framework.

Different methodologies are used for structuring different types of indicators and/or indices. Despite the large variety of frameworks developed so far, many of them are quite similar in their methodological approaches and most is based on causality chains (Ramos *et al.*, 2004 - see Annex I an overview and discussion of these frameworks). DPSIR, developed by the European Environmental Agency, is one of the frameworks for data synthesis and links environmental information using indicators of different categories (*Driving forces*, *Pressure, State, Impacts and Responses*) (RIVM, 1995). This framework will be explained in Part II of this study.

This kind of models of causality chains with the selection of the indicators can be used as a base for a coastal zone environmental management allowing the linkage between environmental and macro-economic models, making it possible to integrate the conservation functions (biodiversity and ecological) with socio-economic development (Casazza *et al.*, 2002). In fact their use has often been applied worldwide to coastal zone management in the last decade. Examples are the work developed by Cooley et al., (1996), Ward *et al.* (1998), Chesapeake Bay Program/USEPA (1999), EEA (1999a), EEA (1999b), USEPA (1999), ME (2001), Casazza *et al.* (2002), Elliott (2002), Jorge *et al.* (2002), Silva and Rodrigues (2002), Nunneri and Hoffmann (2003), Picollo *et al.* (2003) among others. However some of these approaches are only conceptual. Little attention is paid to the difficulties in calculating the indicators of the economic, social and ecological data of the costal system and their spatial visualization and interpretation for future management of the coastal zones. Fully quantified and predictive models will not be possible for many stressors on the system, however decision makers can rely on quantitative relationships and expert judgments (Elliott, 2002).

1.3 COASTAL MANAGEMENT UNITS

A Costal zone management program should have well defined zones that should be subject to management and that can be used as management units. A zoning plan can provide the establishment of smaller areas, which can be applied in a more flexible way (Cicin-Sain and Knecht, 1998). Over the last few decades there has been a move towards identifying these units (McGlashan and Duck, 2002).

The definition of the transition zone between the ocean and terrestrial environment, ocean and coastal zone, and zones (or units) within the coastal areas is sometimes not an easy task. Physical criteria, political boundaries, administrative boundaries, arbitrary distances or selected environment units can and are often used (Clark, 1996).

Boundaries for coastal zone management programs should be located so as to capture and enable resolution of all major coastal issues. Because there is a broad array of possible coastal issues, there is a broad array of possible CZM management boundaries. Most CZM projects use administrative boundaries instead of adopting an ecosystem approach looking at impacts coming from outside the area considered (Belfiore, 2000). Coastal management units are evolving by becoming more inclusive, relying more on processes than administrative boundaries and by incorporating a wider range of expertise in defining relevant areas (McGlashan and Duck, 2002). For example MacDonald *et al.* (2000) developed an ecosystem-based framework for assessing and managing sediment quality conditions in Tampa Bay previously defining management areas. Those areas were defined using interpolated contour lines based on sediment chemistry data and guidelines of potential adverse effects. Picollo *et al.* (2003) used homogenous units for the coastal zone management of the Ligurian region. These subdivisions of the coast corresponded to physiographic units (topographic elements).

Management units can be provided for areas to be specially managed for conservation, research, public safety or public appreciation. Zoning plans must be adapted to specific situations in order to meet the local needs and conditions. Obviously, there will be differences in the type of zones and their arrangement depending on the intensity of use of a particular area as well as the overall size of the area to be zoned (Clark, 1996).

1.4 GIS AND SPATIAL ANALYSIS FOR COASTAL ZONES MANAGEMENT

Scientists have only recently made attempts to transfer information effectively to the end-user, using such high-technology approaches as Geographic Information Systems (GIS) and expert systems models (Cooper, 1994).

GIS are emerging as crucial technology tools for addressing many of the world's most pressing problems, from infrastructure development to environmental and resource management (Sweeney, 1998). GIS provides a convenient tool for resource assessment planning, and management because they carry out analytical functions, are integrative and can be updated. GIS are integrative because they can take data of different formats from different sources. These data are converted into a consistent internal format and scaled within the GIS. The various map layers for a particular area are geometrically registered with one another and with a base map (Clark, 1996).

Different types of information can easily be overlaid, spatial analysis conducted and queries can be perform within one layer or among objects in two or more layers to help identify and assess the effects of human activities on resource systems (Stanbury and Starr, 1999). GIS can provide designating exclusionary areas, high-risk zones, habitat zones, and the like. It can be used to analyse other kinds of information and data derived from remote sensing activities (Cicin-Sain and Knecht, 1998). Resulting overlay maps would give planners and policy makers tools to guide the type and intensity of new developments to choose priority areas for protection or acquisition. It allows more than an educated guess about the intensity and risk of impact that may occur. It does not make the final decision but provides additional information in a readily understood medium so that the decision can be made with a greater degree of confidence (Clark, 1996).

The integration of analytical GIS, Global Positioning Systems (GPS) and remote sensing allows detailed tabulation and visualization of changes to be created over large areas. The result is an effective planning tool and a sound procedure for continued monitoring (O'Regan, 1996), very useful for decision-making processes (Ricketts, 1992).

The appropriate scales to be used in the mapping depend, of course, on both the potential use to which the maps will be put and the nature of the data being mapped (Cicin-Sain and Knecht, 1998).

While advances in expert systems data capture and data storage techniques are forthcoming, coastal scientists and managers themselves have to explore the capabilities of contemporary technologies such as GIS (Ricketts, 1992, Clark, 1996, O'Regan, 1996, Cicin-Sain and Knecht, 1998). The use of key indicators and GIS maps to visualize complex scientific information in natural resources helps to identify particular regions which should receive a higher priority for management and has been well received as a decision support tool (Zandbergen, 1998). Additionally by combining data types, such as socio-political boundaries, bottom types, habitat, species distribution, among other, resource managers can use GIS to make informed management decisions. In this way, GIS provides resource managers with a means to integrate scientific data with prevailing cultural values and traditions (Stanbury and Starr, 1999).

Geostatistical tools, by providing a set of statistical tools for incorporating the spatial and temporal coordinates of observations in data processing, can be integrated in GIS working also as powerful tools for coastal planning purpose. Geostatistics allow the analysis of spatial patterns and the interpolation of the attribute of interest at unsampled locations, assess local and spatial uncertainly about unknown values and integration of secondary data in prediction and simulation algorithms. Geostatistical interpolation methods provide ways to deal with the limitations of other deterministic interpolation methods, like thiessen polygons, inverse distance interpolation or splines. It ensures that the prediction of an attribute value at unsampled points is optimal in terms of the minimization of the expected squared errors of estimation (Burrough and McDonnell, 1998). Geostatistical tools have been largely used in natural resource evaluation like in mining, petroleum, soil science, oceanography, hydrogeology, remote sensing and environmental science (Goovaerts, 1997).

When dealing with environmental, as well as with social, economic or institutional indicators, there is a need to obtain spatially representative samples of the indicator for calculation of average values. By offering geostatistical tools, GIS can assist in making spatially unbiased estimates from geographically distributed measurements. Other types of cartographic illustrations that may be useful in the context of indicator reporting and visualization are reference or index maps, showing the locations of measurement stations (Langaas, 1997). Despite these advantages few studies in coastal management use integrated these spatial analysis and GIS (e.g. Kitsiou, 1998 and Preston, 2002).

1.5 ENVIRONMENTAL MONITORING AND SAMPLING DESIGNS

In coastal zone management studies, estuaries in particular, the monitoring process is fundamental though difficult and time and cost consuming. Estuaries compared with other aquatic ecosystems have several spatial heterogeneities (Kitsiou *et al.,* 2001). In any environmental assessment process a monitoring step should be included to both ensure that mitigation and other countermeasures are carried out and to determine the actual impacts of the action as implemented (Clark, 1996).

Monitoring is a process where repetitive measurements in time and space are recorded to indicate natural variability, and changes in environmental, social and economic parameters. Measuring theses changes contributes to the information base needed by managers to evaluate a plan's effectiveness. Evaluation is analysing information, some of it gained through monitoring, then comparing the results of the analysis against predetermined criteria. A well designed, ongoing monitoring program is fundamental for plan evaluation. (Kay and Alder, 2000). The design of an effective monitoring program depends on the plan's objectives, resources (funding and staff) and available technology. The variables to measure, where to be measured and desired levels of information must be balanced against costs.

Two common types of information used in environmental management are a) baseline information that measures the environmental conditions and status of resources before a project is commenced and b) monitoring information that measure the changes, if any, that occurred after the project was built and operated (Clark, 1996). The statistical reliability of the sampling strategy and parameters used in the baseline surveys and monitoring programs is a key factor.

1.6 SEDIMENT AS A ESTUARINE ENVIRONMENTAL SIGNAL

Sediments have gained prominent attention as a key component of integrative assessment due to complex mixtures of chemicals that commonly characterize contaminated sediments (DelValls *et al.,* 1999). Sediments act as an integrator and amplifier of the concentrations of anthropogenic chemicals in the waters which pass over and transport them, and play an important role in the shallow water estuarine areas. For this reason sediments have been widely used to identify sources of contamination, to measure its extent, and to diagnose the environmental quality of aquatic systems (Luoma, 1990).

The majority of contaminants reaching the costal zones tend to be adsorbed to particulate matter and eventually settle on the water floor, where they can deleteriously affect the sediment-associated community. The degree to which a receiving body is impacted is usually assessed by the analysis of the sediments from the area of concern (Nipper, 2000).

Independent of the geoecological role played by sediments in accumulating or transporting contaminants within a geographic area, the first step is the complete characterization of sedimentary bodies to assess the contamination levels and the distribution of contaminants in order to further identify sources, trends and pathways of pollutants (Queralt *et al.,* 1999).

Although a powerful approach, few studies of estuaries have attempted to explore the relationship between the sediment quality and human activity throughout the coastal zones (e.g. Comeleo *et al*., 1996 and Dauer *et al.,* 2000). Those authors found successful correlations between human pressures like population density, land use or point and non-point loadings, and sediment contamination or benthos integrity.

1.7 WEIGHT-OF-EVIDENCE AND FRAMEWORKS FOR SEDIMENT QUALITY ASSESSMENT

Several methods have been developed for sediment quality assessment for quite a few decades but most of them only focused on one single Line of Evidence (LOE). Line of evidence is a set of information that pertains to an important aspect of the environment (Smith *et al*., 2002). Ramos (1996), presented an overview of these different methods discussing their advantages and drawbacks. However environmental decision-making should be carried out on multiple sets of information or LOE.

Scientific assessments are hampered because of complex interactions between sediment contaminants, biota and contaminants in the overlying water, and the potential for contaminant movement through the aquatic food web. In addition the difficulty surrounding the integration of the various LOE, required to determine the significance of sediment-associated contaminants, has been problematic. This integration is necessary to justify any remedial action, which requires both characterizating ecological hazard as well as the demonstrating a link between exposure and biological effect (Shin and Fong, 1999, Grapentine *et al.,* 2002).

There is no consensus on a single process to evaluate the multiple LOE in sediment quality, a process called Weight of Evident (WOE). There is also no standardized method or regulatory guidance on how to conduct WOE studies. The Sediment Quality Triad (first version in Long and Chapman, 1985), the Consensus-based Approach (Menzie *et al.,* 1996 *fide* Burton *et al.*, 2002), and Considerations Recommended for Relative Chemical Ranking (Swanson and Socha, 1997 *fide* Burton *et al*., 2002) are the only published approaches of which we are aware that provide any degree of guidance on conducting environmental WOE assessments (Burton *et al.,* 2002). The WOE process can help to determine the extent of pollution, its ecological significance, the optimal remedial options and the urgency of corrective actions (Burton *et al.,* 2002).

Sediment Quality Triad (SQT) is the first WOE approach and more largely used and where more improvements and guidelines have been made (e.g. Long and Chapman, 1985; Chapman *et al.,* 1987; Chapman, 1990, Chapman, 1996, Chapman *et al.*, 1997).

The SQT incorporates three essential components or LOE: i) measures to determine the presence and degree of anthropogenic contamination; ii) measures to demonstrate that substances that are present can interfere with the normal functioning of at least some biological organisms tested in the laboratory; iii) assessment of *in situ* alteration of resident biological communities (DelValls *et al*., 1999). Batley *et al*. (2002) discuss the advantages and limitations of observational and investigative lines of these and other LOE.

Ideally sediment chemistry would include direct measurements of bioavailability. However, this is not always possible or necessary provided that other measures of bioavailability are appropriately implemented. Sediment chemistry needs to be combined with bioassays, like acute and non-acute toxicity bioassays to determine the bioavailability fraction of the toxicants. Toxicity bioassays are currently used as a rapid and cost-effective screening tool.

They provide ecologically meaningful information about the threat posed by pollution, while analytical chemistry alone contributes to the interpretation and explanation of toxicity patterns (Beiras *et al.,* 2003). Macroinvertebrate field surveys and laboratory toxicity tests yield different types of information on ecological effects, and both are necessary (Chapman *et al*., 2002). Condition of the ambient benthic community can serve as a reliable and sensitive indicator of potential disturbances resulting from chemical stressors (Hyland *et al.*, 2003). Faunal components of the benthic environment are usually used as integrated indices to analyze the biological indicators. Benthic communities represent powerful tools to reveal disturbance of natural conditions (Casazza *et al.,* 2002).

Single LOE are useful as screening tools but the reality of conflicting results from different lines of evidence requires a WOE assessment for final decision-making (Hall and Giddings 2000 *fide* Chapman *et al.,* 2002). It is difficult to combine the information from these multiple sources into a single measure for decision-making.

There are three different means to assess SQT Weight of Evidence, which are not mutually exclusive: summary indices, multivariate analyses and tabular decision matrices. All require an appropriate reference station or group of stations (Chapman, 1996). Reference sites are similar areas to a test site in regard to physicochemical and biological characteristics and should be the least impacted for purpose of determining unacceptable impairment (Burton *et al.,* 2002).

The first formalized SQT, was based on indices, specifically the development of ratio to reference (RTR) values for each of chemistry, toxicity and benthic community structure (Long and Chapman, 1985; Chapman, 1990). These different variables can also be integrated in one single value with a scoring system. This approach synthesizes integrative data and rank stations and is easily understood by non-scientists (Schmidt *et al.,* 2002). However it is inappropriate to integrate the various LOE findings into one number since important unique information is lost when the LOE ranking are summarized into a single measure, leading to potentially misleading conclusions (Burton *et al.,* 2002).

The SQT has subsequently been refined, removing the RTR approach, and incorporating generic as well as specific sediment quality values and multivariate analysis (Chapman, 1996, Chapman *et al.,* 2002). In order to extract meaningful information from the large and heterogeneous bulk of data generated by the chemical, toxicity and *in situ* benthos, multivariate statistical methods are currently and successfully employed (Shin and Fong 1999; Beiras *et al.*, 2003). These multivariate tools can be Principal Component Analysis (PCA) (e.g. Chapman *et al.,* 1996, Anderson *et al.*, 2001), cluster analysis (e.g. Shin and Fong, 1999), non-metric multidimensional scaling (e.g. DelValls *et al.*, 1998, Beiras *et al.,* 2003), Discriminant Analysis (e.g. Shin and Fong, 1999), correspondence analysis (e.g. Rakocinski *et al.,* 1997), BIO-ENV procedure (e.g. Mucha *et al.,* 2003) among others.

There are different ways and aggregation methods to built indices, that despite data compression and some loss of information, their results are easy to understand and informative. Indices can also be very useful to complement the WOE assessment.

Tabular decision matrices are based on hit/no hit alternatives formatted for decision-making and is neither new nor complex, and comes from one of the few existing frameworks in which Weight of Evidence can be applied. A primarily limitation of this approach as initially proposed (Chapman, 1990) is that it does not explicitly incorporate variance in the quality of the lines of evidence. The assumption is that the data from each Triad component are appropriate. For example, if chemical data are not measured at toxic concentrations and toxicity tests are negative but the community is altered, alteration can not be due to toxic contamination, or the chemical analysis and/or toxicity test may be inappropriate (Chapman, 1996). The hit alternatives are therefore classified according to a logic system probably originated in Koch's postulates (1884) as refered by Chapman *et al.* (2002), that weights the strength of evidence that supports each potential cause (Burton *et al.,* 2002):

i. The adverse effect must be regularly associated with exposure to the stressor;
ii. The stressor must be found in the affected receptor;
iii. The adverse effect must be manifest in unimpaired species, following under controlled experimental conditions;
iv. The stressor (or indicator of exposure) must be found in the experimentally affected species.

The integration of each LOE into a WOE matrix table allows for a comprehensive review and determination of reasonable conclusions on the level of impairment and characterization of stressors. Multivariate analyses can be incorporated in a final tabular decision matrix, as for example Chapman *et al.* (1996) did.

WOE includes both the possible (hazard) and probability (risk) of impacts, beginning with exposure. Information on chemical contamination provides data for assessing exposure, however, biological effects data are required for determining the probability of adverse impacts and their potential magnitude. Effects should be associated with stressor exposure and plausible mechanisms are required to link cause and effects (Chapman *et al.,* 2002). WOE approach can then be seen in an ecological risk assessment (ERA) context, defining WOE as the approach by which measurement endpoints are related to assessment endpoints based on weight, magnitude and concurrence, to determine risk of harm.

Best Professional Judgments (BPJ) should also be taken in to account in WOE framework for contaminated sediments. BPJ comprises the use of expert opinions and judgement based on available data and site and situation specific conditions to determine, for example, environmental status or environmental risk. BPJ can be initiated when there are extensive data but few uncertainties, and when there are few data and many uncertainties. Measurements are weighted by stakeholders based on best professional judgment, relative to the assessment endpoint, the study's quality and design, and on the confidence in the measurement (Menzie *et al.,* 1996 *fide* Chapman *et al.,* 2002).

Sometimes BPJ may be more relevant than statistical comparisons (Chapman *et al.,* 2002). Several more recent studies have been using successfully the WOE approach with BPJ for ecosystem assessment (e.g. Anderson *et al.,* 1998, Albertelli *et al.,* 2003). Albertelli *et al.,* (2003) developed a Coastal Sediment Quality Index based on the SQT incorporating BPJ. The weight of the different components was computed based on an expert judgement according to the Delphi method for better decision-making. The results of each LOE were calculated using the Dashboard freeware software and overall assessment was scored from excellent to critical. This free software allows to present complex relationships between economic, social and environmental issues in a highly communicative format aimed at decision-makers and citizens interested in Sustainable Development (Processdash, 2004). This approach is very interesting and easy to transmit, but still does not allow the association between the indicators, as multivariate analysis does.

The term WOE also suggests that a level of certainty exists with the assessment's conclusion when, in fact, there may continue to be significant uncertainty in the conclusions. This misconception can create significant erosion of the decision-making process linking assessment and remediation, resulting in incorrect management decisions that may be over-or under protective of human and wildlife health. It is apparent that no single WOE approach is appropriate for all assessments of ecosystem impairment, given the wide range of stakeholders concerns and resources availability, and the differences in ecosystems study design, expertise, and execution (Burton *et al.,* 2002). These authors propose a framework that begins by defining key "Certainty Elements" for reliable WOE assessments and accurate decision-making, reducing the role of BPJ and increasing the quantitative assessment components that can be used in sediment quality assessment:

i. Development of a conceptual model, showing linkages of critical receptors (organisms, population or community) and ecosystem quality characteristics;
ii. Explanation of linkages between measurement endpoints responses, direct and indirect with associated spatial/temporal dynamics, and conceptual model components;
iii. Identification of possible natural and anthropogenic stressors with associated exposure dynamics;
iv. Evaluation of appropriate and quantitatively based reference (background) comparison methods;
v. Consideration of advantages and limitations of quantification methods used to integrate LOE;
vi. Consideration of advantages and limitations of each LOE used;
vii. Evaluation of causality criteria used for each LOE during output verification and how they were implemented;
viii. Combining the LOE into a WOE matrix for how they were implemented for interpretation, showing causality linkage in the conceptual model.

All aspects of each WOE, like selection of specific species, toxicological endpoints, WOE categorization criteria, use and number of reference stations, use of background conditions, and the total number of stations needed to characterize the site, should be developed *a priori* in a Problem Formulation/Sampling and Analysis Plan (PF/SAP) that is used as the basis of discussion with regulatory agencies. Development of a PF/SAP (and modification based on stakeholders and regulatory feedback) is essential for the success of the WOE process (Chapman *et al.,* 2002).

1.8 The need for an environmental data management in the Sado Estuary: Portugal

Coastal zone management is no longer restricted to national issues or national policy responses. At European level the 5th Community Program of policy and action in relation to the environment and sustainable development provides for an initiative in response to the council's request for an overall Community strategy on CZM. In this context in 1994 the European Council emphasized the need to develop a European Community strategy for CZM and called on the Commission for drafting such strategy. The exercise aimed at providing results and experiences useful to define and implement a European strategy for CZM based on the "principle of subsidiarity" and taking into account legal, economic and policy instruments, as well as making better use of existing funding schemes. In Portugal, Vale do Lima, Ria de Aveiro and Algarve participate as demonstrative projects. The experience of the demonstration program has underlined, among other things, that reliable and timely information is required within a strategy for collection, processing and diffusion of comparable data and information. This requires the involvement of specialists, in order to analyse raw data and transform them into useful information. The use of spatial analysis, risk assessment, environmental impact assessment, GIS, Gobal Positioning System, indicators, appears particularly promising (Belfiore, 2000). Within the European Union Demonstrative Program on CZM it was also stressed that information must play a central role in the development of a more integrated approach to management. For a better information use in CZM the European Union decided to adopt the indicator framework DPSIR (Doody *et al.*, 1998).

The Water Framework Directive (2000/60/EC - EC, 2000) provides an extra motivation to search for methodologies for ecosystem management as it imposes procedures for the characterization of the ecological and chemical condition of water bodies as well as to clearly define what is the unimpacted state (Silva and Rodrigues, 2002). Other Directives, like urban waste water treatment (91/271/EEC – EC, 1991a), nitrates (91/676/EEC – EC, 1991b), dangerous substances (76/464/EEC – EEC, 1976) and natural habitats and wild fauna and flora (92/43/EEC – EC, 1992), also obligates correct management practices at the European coastal areas.

Coastal nations, like Portugal, have an unprecedented opportunity to set a new course towards sustainable use of the world's coastal and ocean heritage (Cicin-Sain and Knecht,1998).

In Portugal not too many examples of costal zone management exist where integrative studies were developed using different methodologies tools. For example Charneca *et al.* (2002) developed a Geographic Information System tool for environmental evaluation of the

Guadiana River estuary, involving several interdisciplinary teams (River, Estuary, groundwater, ecosystem and socio-economic). Alves *et al.*(2002) developed an integrated management program for the Ria of Aveiro focused on the partnership and public participation to solve the problems and conflicts aiming at the maintenance of social and economic development, as well as the preservation of the natural environmental and the cultural identity. The application of indicators and indices as tools for coastal zone management has also been used in Portugal, although in most cases only in a conceptual way. Painho *et al.* (1996) proposed a conceptual model using indicators of sustainable development for CZM based on coastal management units. Those units can be delineated based on spatial tools that take in to account the ecology, administrative and economic issues. Ramos *et al.* (1998) proposed a list of sustainable indicators to be applied in Portugal, classified according to the *Pressure*, *State*, *Responses* (PSR) indicator framework of the Organization for the Economic Cooperation and Development (OECD) and where the coastal and marine environment was considered. Barbosa and Silva (2001) have delineated and adopted a list of environmental indicators for CZM aiming at the valorisation and protection of the Portuguese coast. Silva and Rodrigues (2002), developed and applied environmental indicators for Tagus Estuary using PSR model.

The Sado Estuary in Portugal is an example where environmental problems are not very well managed owing to the high natural values (most of the estuary is protected as a Natural Reserve) and pressure for development. Many studies have been and still are being developed for this estuary in the different environmental, economic and social components. However few tried to evaluate the global status of the estuary and analyse the information in an integrated and synthetic way aiming at establishing correct data environmental management for transmitting to the different stakeholders including the decision-makers. For example Ramos *et al.* (1998) developed a project aiming at an approach towards the formulation of guidelines for nature conservation and water quality improvement in the framework of integrated river basin planning and management. Within a multi-disciplinary research team biotic and abiotic parameters of the Sado river basin were assessed and analysed in GIS environment. It was a large project but it was not focused on the coastal area and did not integrate the data in indicators or in data management tools. Painho *et al.* (1999), analysed the trend and evolution of the landscape in the protected area of the Sado Estuary in a GIS context. The human pressures, such as urban and industrial land use and transportation network was assessed but no link was made with the estuary quality. Ferreira (2000) examined the ecological quality of Sado Estuary but only regarding eutrophication and spots of sensitive areas using the U.S. National Estuarine Eutrophication Assessment Index. Bricker *et al.* (2003), developed an integrated methodology for the Assessment of Estuarine trophic Status and ranked the eutrophication status of estuaries and coastal areas in the United States and in the Europe, including the Sado Estuary in Portugal. It included quantitative and semi-quantitative components, and used field data, models and expert knowledge to provide PSR indicators. An interesting approach, but only evaluates the eutrophic state. The aim was not to link and integrate the human *Pressures*, which modify the *State* of the environment, and these modifications may have an *Impact* on the ecosystem, as other more demanding indicators frameworks do.

There is a need to urgently developed tools to apply to the Sado Estuary integrating them in a data management framework of social and economic development with the estuary quality. These tools can be used to support decision making by local authorities like municipalities, the Administrative Port of Setúbal and Sesimbra (APSS) and the Natural Reserve of Sado Estuary (RNES).

1.9 OBJECTIVES OF THIS STUDY

The main objective of this work was to develop an estuary environmental management framework using the DPSIR Model, including data collection, data processing and data analysis. The environmental quality of the estuary was assessed through its sediment quality assessment and integrated in a preliminary stage with the human pressures for development. The environmental data management framework, also called along the work EMMSado, was applied to the Sado Estuary. Data management, visualization, processing and analysis was obtained through the combined use of indicators and indices, sampling optimisation techniques, Geographical Information Systems, remote sensing, statistics for spatial data, Global Positioning Systems and expert judgments.

The work developed in this thesis is included in the preliminary planning, one of the first but most important phases of the CZM process, where investigation, collection and data analysis is necessary to enable those responsible to define problems and to identify operational options.

The **specific aims** were:

1 a. To acquire global information about Sado Estuary characterization based on an intensive bibliographic review.

b. To search, through a bibliographic review methodologies for estuary environmental management.

2. To manage and select the environmental indicators for the Sado Estuary using the DPSIR framework.
3. The definition of the environmental management units taking into account parameters of general sediment characterisation and a long spatial sampling strategy, using different methods, and evaluate their robustness.
4. The quantification of the indicators of the *Driving Forces* and *Pressures* categories of DPSIR.
5. To minimize the number of samples using optimisation techniques to define a sampling strategy for monitoring and management.
6. The quantification of sediment quality indicators of *State* and *Impact* categories of DPSIR, including the use of indices to evaluate the sediment contamination and benthos.
7. To define a Weigh of Evidence approach to assess the sediment quality in the management units (and scored them according to their ecology risk), using the Sediment Quality Triad (SQT) approach integrated in a preliminary phase with the *Driving Forces* and *Pressures* of the estuary.

1.10 ASSUMPTIONS

The research assumptions of this work were the following:

1. The Sado Estuary has several environmental problems due to organic and chemical contamination by point and non-point sources; it has high urban, tourist and industrial pressures; it has an important port, fishery, aquaculture and agriculture activities; on the other hand it has high natural values which led to its denomination as a Natural Reserve.
2. It is possible to set up a DPSIR framework to integrate the environmental information for CZM.
3. The GIS together with GPS, remote sensing, and statistics for spatial data are appropriate tools for analysing estuary data.

4. It is possible to delineate adequate sediment homogenous areas as a support tool to Sado estuary monitoring and management.
5. Watershed areas are appropriate units for evaluation of the *Driving forces* and *Pressures* in the estuary.
6. Sediment quality assessment is appropriate to evaluate the *State* and *Impact* of the estuary.
7. It is possible to create a sampling strategy for monitoring that will maximize representativity of zone types and minimize cost of chemical and biological analysis.
8. It is possible to assess the sediment metal contamination using indices.
9. It is possible to assess the benthos using a benthos index that predicts the occurrence of macrobenthic communities, from physical and chemical variables.
10. A Weight of evidence using the Sediment Quality Triad approach is appropriate for the sediment quality assessment.

1.11 GENERAL STRUCTURE OF THIS STUDY

Figure 1.1 shows an outline of the dissertation structure.

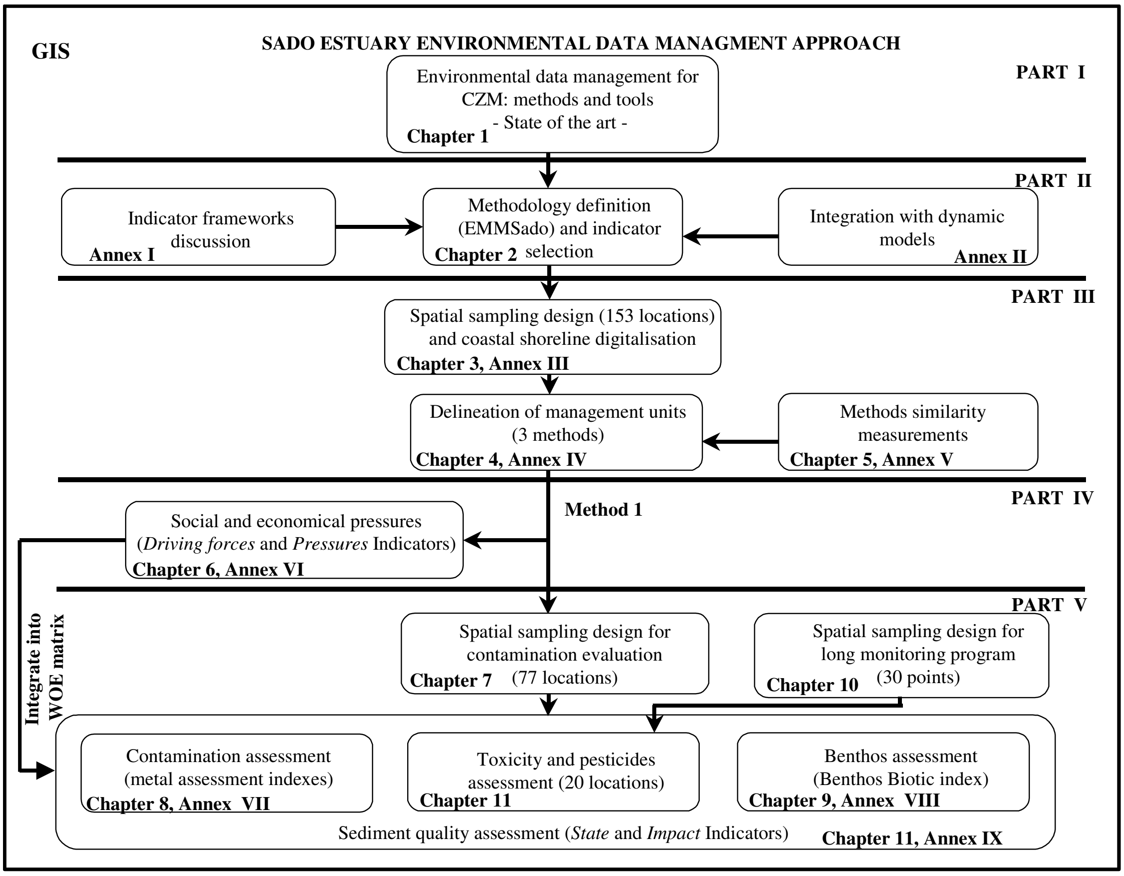

Figure 1.1 – Outline of the dissertation's structure. The part VI (conclusions) is not included.

The thesis is divided mainly in six parts, composed by twelve chapters and nine annexes corresponding to, or based on, articles that are published, under publication, or in preparation. The parts were divided according to the sequence and specific aims fulfillment (see 1.9 Sub-chapter). In the first part, the state of the art of this work research fields was evaluated and further integrated in the different chapters (aim nº 1). On the second part the methodology of EMMSado was defined and the indicators of the DPSIR categories were selected (aim nsº 1 and 2). This part is followed by the delineation of the estuarine management units, support infrastructure of EMMSado (aim nº 3), where the sediment quality will be evaluated. The quantification of the indicators categories of DPSIR framework: *Driving forces* and *Pressures* (aim nº 4), and *State* and *Impact* (aim nsº 5 and 6) went after the first three parts. The overall ecological risk assessment of the management units depicts the final part of this work (aim nº 7). The following papers compose then the six parts:

PART I – Global Introduction

Chapter 1: State of the art, objectives, assumptions and structure of the thesis.

PART II – Methodology definition and indicator selection for DPSIR

Chapter 2: Caeiro, S., Costa, M. H., Painho, M. and Ramos, T. B. (2002) Sado Estuary Environmental Management: A GIS Approach. In: *Proceedings of Euroworkshop ECO-GEOWATER GI and Water Resources Assessment*, GISIG, 9 – 13 July, Oxford, England. http://www.gisig.it/eco-geowater/VirtualPConference. pp. 1 – 13.

PART III – Delineation of estuarine management units

Chapter 3: Caeiro, S., Goovaerts, P., Painho, M., Costa, M. H. and Sousa, S. (2003). Spatial sampling design for sediment quality assessment in estuaries. *Environmental Modelling and Software* 18(**10**) 853 - 859.

Chapter 4: Caeiro, S., Goovaerts, P., Painho, M., Costa, M. H. (2003) Delineation of estuarine management areas using multivariate geostatistics: the case of Sado Estuary. *Environmental Science and Technology* 37(**18**). *4052 – 4059.*

Chapter 5: Caeiro, S., Sousa, S., Painho, M. (2003). Map similarity measurement and its application to Sado Estuary. *Finisterra* 75 (*in press*).

PART IV- Social and economical pressures

Chapter 6: Caeiro, S., Mourão, I., Costa, M. H., Ramos, T., Painho, P. and Sousa, S. (2004). Application of the DPSIR model to the Sado Estuary in a GIS context – Social and

Economical Pressure. In: Toppen, F., Prostacos, P. (Ed.) *Proceedings of 7th AGILE Conference on Geographic Information Science,* AGILE, Greece, Heraklion, 29 April - 1 May of 2004. pp. 391 - 402.

PART V- Sediment quality assessment

Chapter 7: Caeiro, S., Nunes, L., Goovaerts, P., Costa, H., Cunha, M. C., Painho, M., Ribeiro, L. (2004). Optimisation of an estuarine monitoring program: selecting the best spatial distribution. In: A. Soares, J. Gomez-Hernandez, and R. Froidevaux, (Ed.) *GeoENV IV Geostatistical for Environmental Applications*. Kluwer Academic Press. Dordrecht. pp. 355 - 366.

Chapter 8: Caeiro, S., Costa, M. H., Ramos, T. B., Fernandes, L., Silveira, N., Coimbra, A., Medeiros, G. and Painho, M. (2003). Assessing Sediment Heavy Metals Contamination in Sado Estuary: A Index Analysis Approach. In: *Abstract proceedings of CICTA 2003 – 5th Iberian and 2nd Iberoamerican Congress of Environmental Contamination and Toxicology. Environmental Problems in an Iberoamerican Context,* CICTA, 22 – 24 September 2003, Porto, Portugal. pp. 147 (submitted to *Ecological Indicators*).

Chapter 9: Caeiro, S., Costa, M. H., Goovaerts, P., and Martins, F. Benthic biotope Index development for Sado Estuary: Portugal. (submitted to *Marine Environmental Research*).

Chapter 10: Caeiro, S., Nunes, L., Goovaerts, P., Painho, M. and Costa, M. H. Optimisation of Sediment Estuarine Monitoring Program Using Contamination Data. In: *Proceedings of 5th International Symposium on GIS and Computer Cartography for Coastal Zone Managemen*t, GISIG, 16 – 18 October 2003, Genoa, Italy, http://www.gisig.it/coastgis/. pp. 1 – 9.

Chapter 11: Caeiro, S., Costa, M. H., DelValls, A., Repolho, T., Gonçalves, M., Mosca, A., Coimbra, A. P. and Painho, M. Weight of Evidence to assess sediment quality in management units: application to Sado Estuary Portugal. In: *Long abstract proceedings of the 4th Workshop Harmonization of impact assessment tools for sediment and dredged materials*, SedNet, AZTI and II QAB – CSIC, 10 – 11 June 2004, San Sebastian, Spain. pp. 64 - 68 (*paper in preparation*).

PART VI - Global conclusions

Chapter 12: Conclusions, limitations and future developments.

ANNEXES

Annex I: Ramos, T. B., Caeiro, S. and Melo, J. J. (2004). Environmental Indicators Frameworks to Design and assess Environmental Monitoring Programs. *Impact Assessment and Project Appraisal Journal.* 22(**1**) 46 – 62.

Annex II: Painho, M., Sena, R., Caeiro, S., Martins, F., Costa, M. H. and Neves, R. (2002). Integration of numerical models in geographic databases: the case of Sado Estuary management. In: Clucjie, I. D., Han, D., Davis, J.P. and Heslop, S. (ed.) *Proceeding of 5th Hydroinformatic 2002*, International Water Association, 1- 5 July, Cardiff, England. pp. 1239 – 1245.

Annex III: Support information of Chapter 3

Annex IV: Support information of Chapter 4

Annex V: Sousa, S., Caeiro, S. and Painho, M. (2002). Assessment of map similarity of categorical maps using *kappa* statistics. In: Sousa, A. *et al.,* (ed.). *Proceedings of ESIG 2002*. VII Encontro de Utilizadores de Informação, ESIG, 13 – 15 Novembro. Tagus park. http://www.igeo.pt/IGEO/portugues/servicos/biblioteca/PublicacoesIGP_files/esig_2002/pagina_interior.html. pp. 1 – 6.

Caeiro, S., Sousa, S., Pontius, Jr. R. G. and Painho, M. (2003). Sado Estuary management areas: Hard versus Soft Classification Maps Comparison. In: *Proceedings of 5th International Symposium on GIS and Computer Cartography for Coastal Zone Management*, GISIG, 16 – 18 October 2003, Genova, Italy, http://www.gisig.it/coastgis/. pp. 1 – 9.

Annex VI: Support information of Chapter 6

Annex VII: Support information of Chapter 8

Annex VIII: Support information of Chapter 9

Annex IX: Support information of Chapter 11.

This thesis was integrated in a research Project approved by the Portuguese Science and Technology Foundation and POCTI (Research Project nº POCTI/BSE 35137/99) and financed by FEDER. Owing to its interdisciplinary characteristics different institutions composed this Project: New University of Lisbon (UNL) – Department of Environmental Science and Engineering/IMAR, Chemistry Department/Environmental Biotechnology Unit and Institute for Statistics and Information Management (ISEGI); Distance Learning University – Department of Exact Sciences and Technologies and Controlab Laboratory. Also other institutions, not financed by this Project, have collaborated in this research: University

of Algarve (Faculty of Marine and Environmental Science and Higher School of Technology); the Sado Estuary Natural Reserve (RNES) and the Administration Port of Setúbal and Sesimbra (APSS). In addition several international consultants participated on the project.

In Part I, **Chapter 1**, the present section, a general overview of methods and tools used in Coastal zone management is discussed.

In Part II the methodology for the EMMSado is described. The application of the DPSIR framework is explained and the selected indicators for each category are listed (**Chapter 2**). In **Annex I** a complete discussion about the existing indicator frameworks and their advantages and drawbacks is presented in a scientific journal article. This article also gives an example of their application and usefulness in environmental monitoring programs in a Sado Coastal infrastructure. This work was conducted with the collaboration of University of Algarve. The EMMSado methodology can and should allow the integration of hydrodynamic models in the GIS. This integration is still under research but can be very useful for *Impact* assessment and *Responses* measures forecast (**Annex II –** integration conducted by ISEGI team with a numerical model developed by a team of University of Algarve). In this chapter it is explained that the final objective of EMMSado, is the environmental management actions, including the indicator's quantification of *Response* category. However this phase was not included in this thesis.

In Part III the steps for delineation of the management units for EMMSado are provided. The spatial sampling design used for the delineation of the management units is explained in **Chapter 3** and support information in **Annex III**. The estuarine boundary (coastal shoreline) definition, conducted in collaboration with ISEGI team, is also explained in this chapter. The delineation of the environmental management units (also called homogenous areas along the text) was computed using the sediment data (fine fraction, redox potential and organic matter) of a first 153 locations data sampling design (sampled from October 2000 to January 2001). The IMAR/UNL team conducted the sampling campaign, with the collaboration of RNES, and the laboratory work. Three methods using multivariate geostatistics tools were used for the management unit's computation (**Chapter 4,** and support information in **Annex IV**). These methods were compared using different map similarity measurements (**Chapter 5**) and the most appropriate one was chosen (method 1). Since in the article of this chapter it was not possible to explain all the measurements used for map comparison, that explanation is shown in **Annex V** in two conference papers. The map similarities procedures were also conducted in collaboration with ISEGI team.

In Parts IV and V is when the indicators of the first four DPSIR categories are developed and evaluated, based on which the management of the estuary can be conducted. **Chapter 6** in Part IV (and support information in **Annex VI**) is focussed on a preliminary indicator evaluation of *Driving forces* and *Pressure* categories. On this preliminary stage the terrestrial indicators were only evaluated in the Setúbal sub watershed. The main human pressures of the estuary are located in this area. The data of this chapter will be integrated with Part V.

In Part V all the different steps for sediment quality assessment were conducted, i.e. the quantification of the *State* (sediment chemistry) and *Impact* (benthos disturbance and toxicity) categories of DPSIR framework in the management units. Only these indicators of sediment quality assessment were measured from the *State* and *Impact* indicators list shown in Chapter 2. These indicators were considered the ones with more feasibility and relevancy. Since the analyses of the sediment contaminant's concentrations in the 153 locations, were very expensive, an optimisation model was used to select the best sampling number and spatial distribution (**Chapter 7**). A team from the University of Algarve developed the model used. In the resulting reduced number of locations (77, sampled in the campaign of 2000/2001) a chemical team from the Controlab Laboratory determined the concentrations of the more important heavy metals and metalloids[♦], taking into account earlier work conducted in the estuary and estuarine pollution sources. Their results were evaluated, aggregated and discussed using different indices for sediment contamination evaluation (**Chapter 8** and support information in **Annex VII**). On the same 77 sampling points the benthos community's structure disturbance was extrapolated. This extrapolation was developed using an index based on a benthos survey conducted 15 years ago by other authors. Hydrodynamic parameters simulated using a hydrodynamic model (the same presented in Annex II) and our data on sediment characteristics were used as input data of the index (**Chapter 9** and support information in **Annex VIII**). The third Sediment Quality Triad component, the toxicity bioassays, were only possible to be conducted in a more reduced number of samples due to budget and time constrains. The optimisation model was used again to choose the best

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[♦] The heavy metal concentrations were measured in 78 sampling points, one more location was measured due to an logistic error.

sampling points for the toxicity tests. A 30 sampling locations design strategy was defined as a network to be used as a long-term monitoring program within EMMSado (**Chapter 10**). Due to logistic problems it was only possible to conduct the toxicity bioassays in 19 of the 30 sampling network, representative of each management area. The IMAR/UNL team conducted the sampling campaign, with the collaboration of RNES, and the bioassays work. In these same 20 locations (representative of each management unit), the chemical team from New University of Lisbon determined 14 organochlorine pesticides concentrations. Organochlorine pesticides are of primary concern in sediment and aquatic biota due to their hydrophobic characteristics and being heavily used since the 1940s. Finally the Weight of Evidence approach was used to assess the sediment quality assessment using the data of the three SQT components (chemistry, benthos and toxicity). In the WOE approach indicators of the *Driving Forces* and *Pressures* categories defined in Chapter 6 were integrated for a better overall assessment of the management units (**Chapter 11** and support information in **Annex IX**).

The main conclusions and future developments are discussed in **Chapter 12** Part VI.

Since the structure of this thesis is composed by independent published or under publication articles some methodologies and results framing had to be repeated, most of the times owing to referee requests.

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PART II

METHODOLOGY DEFINITION AND INDICATOR SELECTION FOR DPSIR

CHAPTER 2 – SADO ESTUARY ENVIRONMENTAL MANAGEMENT: A GIS APPROACH

SADO ESTUARY ENVIRONMENTAL MANAGEMENT: A GIS APPROACH

Caeiro, S., Costa, M. H., Painho, M. and Ramos, T. B. (2002)

Proceedings of *Euroworkshop ECO-GEOWATER "GI and Water Resources Assessment"*, 9-13 Julho, Oxford, England. http://www.gisig.it/eco-geowater/VirtualPConference. pp. 1 – 13.

ABSTRACT

Coasts and estuaries are typical environments in which human impacts have led to a whole range of changes with considerable variation in their degree of impact. The simultaneous occurrence of attractiveness for human use and natural value has lead to policy conflicts between conservation and development. The Sado Estuary in Portugal is an example where these kinds of conflicts exist because of its location near industrialised urban zones and its designation as a Natural Reserve. Therefore, it has become quite inevitable to implement a model of environmental management based on methodologies that enable the evaluation of the coastal zone processes of the Sado Estuary. The aim of this paper is to present a methodology for a coastal zone environmental management system applied to the Sado Estuary. This ongoing methodology is based on the DPSIR model and is developed within the context of a Geographic Information System. DPSIR, developed by the European Environmental Agency, provides a framework for data synthesis and links environmental information using indicators. The selected indicators for the specific case of the Sado Estuary are also described in detail. The methodology proposed can be used for the assessment of environmental conditions, development of management plans and design of specific restoration/conservation actions to be carried out by the responsible institutions like regional governments.

KEYWORDS: Environmental management, estuaries, DPSIR Model, indicators, GIS, sediment quality.

2.1 INTRODUCTION

The coast is a highly populated area, usually used as a place to live or for leisure and also where industrial and port activities are in a constant development. As a consequence intense pressure and demands from various sectors of the community occur on the ecosystem. These pressures have the potential to cause change and environmental degradation, if not carefully managed. It is then necessary to operate under a system of management, by which control is made on this the activities. They must be managed in such a way as to minimise the detrimental effects on the environment, and to ensure that important habitats are not perturbated. Coastal zone management represents therefore a dynamic process which develops and implements a co-ordinated strategy to allocate resources to achieve the conservation and sustainable multiple use of the coastal zone (French, 1997). The importance of understanding the dynamic nature of the coastal zone and the links between their habitats and the role for human activity in changing its structure and function is central to achieve that goal of management (Doody, 2001).

The Sado Estuary in Portugal is an example where environmental problems are not very well managed. It becomes thus necessary to develop a model to accurately evaluate the environmental quality and identify and manage the conflicts for conservation of this coastal ecosystem. In such a stressor-response model it is impossible to completely characterize all the variables, so a selected set of measurements should be made to reflect the most critical components (Fisher *et al.*, 2001). Indicators are an excellent way of representing the environmental components avoiding the measurement of too many parameters. UNEP/RIVM (1994), defines an indicator as a piece of information which is a part of a specific management process and can be compared with the objectives of that management process and has been assigned a significance beyond its face value. Indicators are often adopted to avoid and reduce the complexity of environmental data. In general, indicators are easily quantified and delineated from already described information in protective goods like environmental compartments and are adequate to assess what is called ecosystem health (Costanza, 1992). The use of environmental quality indicators also appears as a good tool for processing, analysis and transmission of raw environmental information to technicians, decision-makers, managers or the public in general.

Different methodologies are used for structuring the different types of indicators and/or indices. Despite the large variety of frameworks developed, many of them are quite similar in their methodological approaches and a good number is based on causality chains (Ramos *et al.*, 2004). DPSIR, developed by the European Environmental Agency, is one of the frameworks for data synthesis and links environmental information using indicators of different categories (*Driving Forces*, *Pressure*, *State*, *Impacts* and *Responses*). This framework can be used as a base for a coastal zone environmental management allowing the linkage between environmental and macro-economic models, making it possible to integrate the conservation functions (biodiversity and ecological) with socio-economic development (RIVM, 1995).

The aim of this paper is to present an ongoing methodology for a coastal zone environmental management system applied to the Sado Estuary. This methodology is based on the DPSIR model and is developed within the context of a Geographic Information System. This paper also describes in more detail the indicators selected for this framework.

2.2 THE STUDY AREA

The Sado Estuary is the second largest in Portugal with an area of approximately 24,000 ha. It is located in the West Coast of Portugal, within a boundary box set by the coordinates of 8º42' W 38º25' N and 8º57' W 38º32' N. The estuary comprises the Northern and the Southern Channels, partially separated by intertidal sandbanks. Most of the water exchange is made through the southern Channel, which reaches a depth of 25 meters, whereas the Northern Channel's maximal depth is generally 10 m. The estuary is linked to the ocean by a narrow and deep channel (maximal depth of 50 m) that makes a major contribution to the general pattern of the estuarine circulation (Neves, 1986). Most of the estuary, except for the city of Setúbal, its port and a considerable part of its surrounding area, is classified as a Nature Reserve (D.L. nº 430/80). It is internationally protected by the Ramsar Convention due to high biodiversity values, with a great variety of animal and plant species (Caeiro *et al.*, 2002).

The Sado estuary is subject to intensive land use practices and plays an important role in the local and national economy. There are many industries of different types as well as hazardous waste landfills mainly on the northern margin of the estuary (Catarino *et al.*, 1987, Ferreira, 1998). Furthermore the harbour-associated activities and the city of Setúbal, along with the mines on the Sado watershed, use the estuary for waste disposal purpose without suitable treatment. In the remaining areas around the estuary, intensive farming, mostly rice fields, is the main land use (about 4000 ha), together with an increasingly intensive fish farms (about 1000 ha) (Painho *et al*, 1996). Some of these activities have negative effects on water, sediment and biotic communities namely because they discharge to the estuary contaminants like heavy metals, hydrocarbons, pesticides and fertilisers (IH, 1993, Caeiro, 1996, Ferreira, 1998 and Cerejeira *et al.*, 1999). Inside the estuary, relatively intensive fisheries are conducted for fish (*e.g. Mullus surmuletus, Liza aurata*, *Spondyliosoma cantharus*, *Dicentrarchus labrax*, and *Sparus aurata*) (Morais, 1994), molluscs (*e.g. Ensis siliqua*, *Callista chione*, *Chamelea striatula*, *Sepia officinalis* and *Donax spp*.) (Dias *et al.,* 1994) and bait (*Marphysa sanguinea*) (Dias, 1994).

The Tróia Peninsula offers areas with coastal recreation facilities and is used for a range of leisure interests that have recently increased at a rapid pace. At the present moment there are expansions of tourism complexes that result in several pressures on the estuary (Andrade *et al*., 1998).

The intensification of industrial activity and harbour development are claiming areas along the northern bank of the estuary and increasing the stress already imposed as well as changing the sedimentary environment. Also the actual intent of building new ports and dredging the North Channel of the estuary could also cause serious environmental impact (Costa *et al.* 1998, HIDROMODE, 1998, Rodrigues and Quintino, 2002).

Vasconcelos *et al.* (1999) discussed a pressure increase on the North bank of the estuary, due to the attraction of the city of Setúbal. These authors also showed that the establishment of the Natural Reserve seemed to have kept industrial uses away from the protected area, though the expansion of urban land inside the Protected Area might constitute a threat if not properly controlled. In the near future, the northern part of the Reserve will probably be under demographic pressure and will require urgent management measures. Difficulties of Reserve authorities in managing urban growth are reflected in the higher urban growth rate inside the protected area boundary when compared with its surroundings. This is probably due to the fact that numerous official bodies are responsible for landuse planning in the Reserve area, causing, at times, management bottlenecks.

2.3 THE APPLICATION OF THE DPSIR MODEL TO THE SADO ESTUARY

The DPSIR model organizes information in five different compartments: *Driving forces, Pressure, State, Impacts and Responses* (Fig. 2.1). *Driving forces*, are the underlying causes of environmental problems. They refer to the needs of individuals and institutions, which lead to activities that exert *Pressures* on the environment. For example, the human need for food is a driving force that motivates fishing that implies the harvest of fish resources. The "intensity" of the pressure depends on the nature and extension of the driving forces and also on other factors which shape human interaction with ecological systems. These pressures modify the *State* of the environment (*e.g.* change in sediment or water quality, fish populations), and these modifications may have an *Impact* on ecosystems and on human well-being. Undesirable impacts lead to a *Response* from society that results in the formulation of an environmental policy. The policy responses lead to changes in the DPSIR chain. Depending on the results achieved, further responses are formulated (RIVM, 1995 and Antunes and Santos, 1999).

This kinf of indicators framework is useful because it leads both scientists and policy makers to think in terms of causality chains. DPSIR is being used with success namely in European Environmental Reports, and the State and Pressure of the Marine and Coastal Mediterranean Environment report developed by European Environmental Agency (EEA, 1999a, 1999b), as well as in other studies applied to oceans (Antunes and Santos, 1999) and coastal zones (Turner and Salomons, 1999, among others).

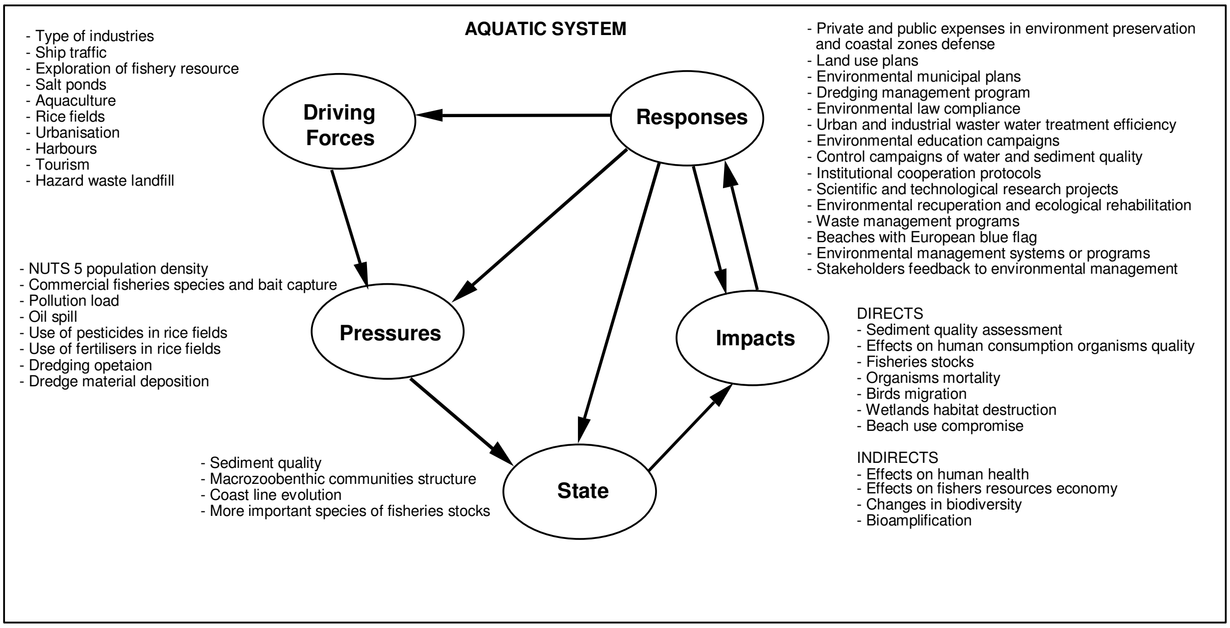

Figure 2.1 – DPSIR Model applied to the Sado Estuary (adapted from Caeiro *et al.*, 2002).

The identification and assessment of problems related to coastal zone environmental management requires the definition of a set of indicators aimed at the different parts of the framework. Some of the most important criteria for indicator selection are (Ramos *et al.*, 2004):

- social and environmental relevance;
- appropriateness of scales (temporal and spatial);
- acceptable levels of uncertainty;
- minimal environmental impact of sampling process itself;
- provide a representative picture of marine environmental conditions;
- be simple, easy to interpret and be able to show trends over time;
- be responsive to change in the marine environment and related human activities;
- data collection methods comparable with other data sets;
- give early warning about irreversible trends where possible;
- be capable of being updated at regular intervals;
- have a target level or threshold against which to compare it so that users are able to assess the significance of the values associated with it;
- readily available or made available at a reasonable cost/benefit ratio;
- be theoretically well founded in technical and scientific terms.

There is a rich set of sources for developing and discussing environmental indicators and indices selection, concepts and criteria. For further information see for example EEA (1996), HMSO (1996), Ramos (1996), UNDPCSD (1996), USEPA/FSU (1996a, 1996b, 1996c), Ramos *et al*. (1998), Caeiro *et al*. (1999) and Jackson *et al.* (2000).

Applying the DPSIR framework to the Sado Estuary means finding an appropriate set of indicators for each compartment (Fig. 2.1). This was obtained by comparing optimal indicator criteria against an extensive data search on Sado Estuary environmental characterisation including: hydrography, geomorphology, contamination sources, water, sediment and biota quality, biodiversity, land use conflicts, social and economy aspects, land use planning (for example, Catarino *et al*., 1987, IH, 1993, Rodrigues and Quintino, 1993, Dias, 1994, Dias *et al.*, 1994, Morais, 1994, Caeiro, 1996, Painho *et al.*, 1996, Andrade *et al*., 1998, Ferreira, 1998, Cerejeira *et al*., 1999, Vasconcelos *et al.*, 1999, Rodrigues and Quintino, 2002, among much other studies).

In the *Driving forces* category the indicator selection was based on the human activities that have impact in the estuary. The following is a list of the resulting indicators and related units:

- urbanisation in the zones near the estuary (km^2 of influence area occupied by urban zones);

- type of industry (number of establishments per industry type/ km coastal line);
- hazardous waste landfills in the zones near the estuary (km^2);
- rice fields (km^2);
- salt-pans (km^2);
- aquaculture (km^2);
- exploratory activities of fishery resources (number of fishing licensed boats per harbour/year);
- commercial, repairing and building harbours (km of coastal line occupied by harbour zones or number of harbours);
- ship traffic (traffic of ships per harbour - ships/year);
- Tourism development in the zones bordering the estuary (km^2 of influence area occupied by tourism facilities).

In the *Pressures* category the indicators selected and related units were based on the human activities previously defined:

- NUTS5 (administrative unit one level down of the city - NUTS4) population density in the zones near the estuary - (number/km^2/year);
- Oil spill (kg/year or nº of spills occurrence/ year);
- Use of pesticides in rice fields (t/ha/year);
- Use of fertilisers in rice fields (t/ha/year);
- Commercial fisheries species and bait capture (thousands of tones live weight/year);
- Dredging operation and inert extraction (m^3/year);
- Dredged material deposition (m^3/year);
- Pollution loads measured through:
  - discharges of industrial and domestic wastewater without suitable treatment (m^3/year or g contaminant/l);
  - solid waste discharges (t/year);
  - water runoff (non-point source like for example agriculture) obtained by modeling estimation (m^3/year).

Due to the pressures listed above the *State* of the Sado Estuary should be analysed through the following indicators and related units:

- Sediment quality measured through the following indicators:
  - organic matter (%);
  - sediment granulometry (% of fine fraction, sand and gravel);
  - redox potential (mV);
  - heavy metals: Zn, Cu, Cd, Pb, Hg, As and Cr (μg/g);
  - Polyaromatic Hydrocarbons (PAH) (μg/g);
  - Polychlorinated biphenyls (PCB) (μg/g);
  - organochlorine pesticides (μg/g);
  - Tributyltin (TBT) (μg/g);
  - faecal contamination indicator (MPN/100 ml);
- Macrozoobenthic community structure (assessed through species richness, abundance, biomass, species diversity, evenness, *k*-dominance curves among others);
- Coastline evolution (cm of coastaline or cm^2 area changed /year);
- More important estuarine species of fisheries stocks (ton of fresh biomass/year).

The *Impacts* and related units which are a consequence of the state of the environment of the aquatic system are:

Direct Impacts

- Sediment quality assessment (*e.g.* toxicity tests, macrozoobenthic communities disturbance assessment, Sediment Background Approach, Sediment Quality Triad Approach, Equilibrium Partitioning Approach);
- Effects on the quality of organisms used in human diet measured through the following indicators:
  - presence of indicators of faecal contamination in bivalvia (MPN indicator of faecal contamination/g fresh weight);
  - ictiofauna deformations (% deformations in vertebres or ural plates);
  - molluscs and crustaceans contaminants bioaccumulation (μg contaminant/g fresh weight;
  - bivalvia biotoxines accumulation (μg biotoxine /100 g fresh weight);
- Effects on fisheries stocks (% estuarine fisheries stocks below the minimum biological acceptable level – HMSO, 1996);
- Organisms mortality - fish, birds and mammalian (number of deaths/species/year caused

by anthropogenic perturbations);

- Birds migration pattern changed due to anthropogenic actions (annual census);
- Wetlands habitat destruction (% total wetland area destroyed or disappeared/year);
- Beach uses compromise (number of beaches with bad water quality (EU classification)/year);

Indirect Impacts

- Effects on human health (symptom occurrence of gastro-enteritis associated with swimmers and/or consumers by 1000 individuals; symptom occurrence of dermatoses and/or mycoses associated with swimmers by 1000 individuals; fatal cases of meningitis associated with swimmers and/or consumers by 1000 individuals/year);
- Changes in biodiversity - species and habitats (n/year);
- Bioamplification (organism contaminant concentration in trophic level n / organism contaminant concentration in trophic level $n - 1$).

Owing to all this 4 categories the *Responses* and related units of Sado ecosystem are:

- Private and public expenses in environment preservation and coastal zones defense (EURO/year);
- Land use plans (e.g. Regional, Municipal, Sado Estuary Natural Reserve, Sado Watershed, Sado-Sines Costal Zone, Setúbal Riverine land use plans and Environmental municipal plans (% implemented or in implementation, or % regulatory requirements enforced);
- Environmental law compliance - e.g. Nitrate, Water Framework and Sewage Sludge Directives (yes/no or % regulatory requirements enforced);
- Dredging management program (% m^3 of dredged material under management program);
- Urban and industrial waste water treatment efficiency (% BOD or other contaminant removal);
- Waste management program (e.g. % of solid waste dumped in the estuary or collected in appropriate containers);
- Environmental education and awareness campaigns (nº campaigns/year or nº of citizens involved in voluntary monitoring programs/year);
- Control campaigns of water and sediment quality (nº/year);
- Institutional cooperation protocols (nº/year);

- Scientific and technological research projects (nº/year);
- Environmental restoration and ecological rehabilitation projects (nº/year);
- Beaches with European blue flag (nº candidate beaches/year);
- Environmental management systems or programs in private and public organization (nº/year);
- Stakeholders feedback to estuary environmental management (nº contacts received in the estuary environmental management focal point – e.g. Sado Estuary Natural Reserve/year).

In the proposed model, the *state* and Direct *Impacts* of the Estuary are mostly evaluated through the sediment and benthos compartment since sediment is a compartment where contaminants such as heavy metals or organic compounds tend to accumulate first (French, 1997). Many authors have been using sediment to monitor aquatic contamination, showing great advantages when compared to traditional water sampling (*e.g.* Wilson, 1988; Elliot and Mcmanus 1989). In most of the cases the sediment contaminant levels suffer short variations for short time periods reflecting the average conditions of month periods (Luoma, 1990). Since contaminants that enter in the estuarine and marine ecosystems eventually bind to sediment particles and are deposited on the bottom, we propose an emphasis on benthic organisms as a primary means of assessing ecosystem response. Of particular importance are the macrobenthic invertebrates because of their short longevity, sedentary life styles, proximity to sediments, influence on sedimentary processes and trophic importance (Diaz, 1992). That is why macrobenthic communities structure is such an important indicator to assess the state of Sado Estuary. Besides these advantages, studying the state of the estuary mainly based on the sediment and benthos compartment also turns this methodology easier, faster and human and financial resource saving. These are essential factors to an efficient environmental management of coastal areas.

A more in-depth analysis of the indicators listed above shows the difficulties that arise in the application of the DPSIR framework to complex environmental problems, as is the case of marine resources. These difficulties can be due to several factors such as (UNEP/RIVM, 1994, Ramos, 1996 and Antunes and Santos, 1999):

- several causes contributing to a single effect;
- multiple effects resulting from a single pressure;
- obscure the more complex relationships in ecosystems and the interactions among sub-

systems (e.g. socio-economic and ecological);
- indirect, synergistic or cumulative effects;
- find the mathematical equations that better represent the parameters behavior;
- lack of available data.

One of the difficulties is to assess whether a specific observed *pressure* causes the environmental changes. But these causality frameworks should not attempt to make on-to-one linkages between specific *pressures*, environmental changes and *responses*. The *state* of the environment depends on the total *impacts* of multiple *pressures*. One way to deal with this complexity is to avoid unique linkages, and try to adopt an integrated approach, that relates different indicators as clusters with multiple aspects that interact with each other (Ramos *et al.*, 2004).

Also, Greeuw *et al.* (2001), stated that in this framework, a *pressure* in one situation might be an *impact* or a *response* in another. However, this framework provides a basis for identification of information needs and for problem assessment.

The indicators belonging to all these categories, namely the sediment chemistry and biota quality indicators could be composed by classification and aggregation of one or more indicators, by means of precise mathematical models or heuristic algorithms (Melo *et al.*, 1996). Most of these aggregations were already tested and are available in literature. Examples of these kinds of indices are Pollution Index, Biological Quality Index, Biotic Index, Pollution Load Index among others. For example the Pollution Load Index is calculated by the aggregation of contaminants like heavy metals or polyaromatic hydrocarbons. For a review of these and other indices see for example Wilson and Jeffrey (1994) and Ramos (1996).

To avoid a too complex and resource-demanding data acquisition the indicators could be scored according to a qualitative expertise-based classification of their relevancy and feasibility. The relevancy classification covers: i) technical and scientific importance, ii) synthesis capacity and iii) usefulness for communicating and reporting. The feasibility classification covers sensibility, robustness, cost and operability of the determination methods. In a first phase diagnose only the indicators with the highest classification can be included. The other indicators should be considered dependent of the evaluation of the first results. More details about this scoring can be found in Ramos *et al*. (2004) (see Annex I).

2.4 Description of Sado Estuary environmental management methodology (EMMSado)

The methodology proposed for the environmental management system applied to Sado estuary supported on the DPISR framework, is based on identifying, representing and characterizing homogeneous environmental areas (management units) for the aquatic system quality assessment (see Fig. 2.2). On each of these management units DPSIR indicators are going to be quantified. For quantification of the human activities and pressures indicators located in the terrestrial zone, boundaries are drawn based on administrative limits that are in the neighbour area of the Sado Estuary (NUTS 5 administrative units or watershed limits).

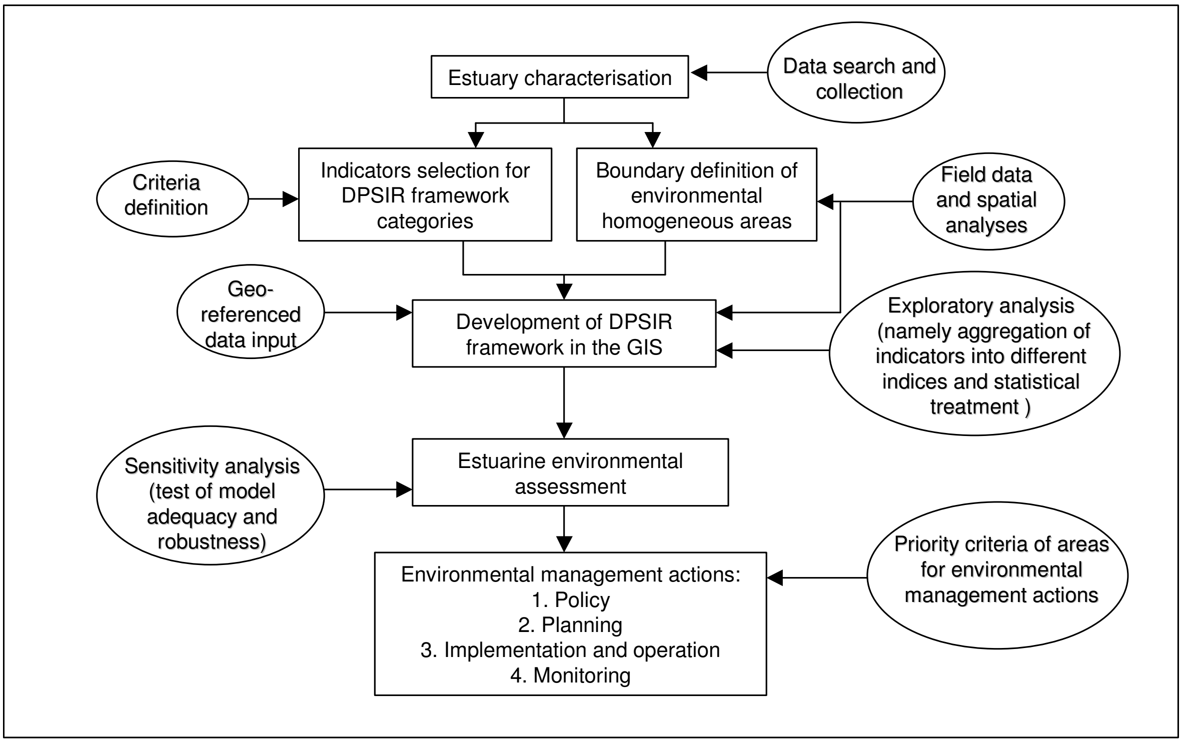

Figure. 2.2 – Methodology for the Sado Estuary environmental management framework (adapted from Caeiro *et al.*, 2002).

For the purpose of management unit's delineation, a first extensive campaign with sediment locations was sampled for analysis of properties of general characterisation: sediment Fine Fraction content (FF), Total Organic Matter (TOM), and Redox Potential (Eh). These key ecological parameters explain main variations in the type and behaviour of benthic organisms as well as contaminant mobility/accumulation (Rodrigues and Quintino, 1993). A systematic unaligned sampling design should be used based on prior information on the spatial variation of sediment granulometry (Caeiro *et al.*, 2003b – see Chapter 3).

With this grid an extensive campaign was sample and the data thus acquired used to draw homogeneous areas for Sado Estuary (future management units) after interpolation and aggregation methods. These homogenous areas were delineated based on grouping individual sampling sites with similar physicochemical properties and geographically close, i.e. using multivariate geostatistics tools (Caeiro *et al.*2003a – see Chapter 4). The management units were overlaid within the estuary coastline (Caeiro *et al.,* 2003b – see Chapter 3) using ArcGIS® GIS software (Fig. 2.3). Aerial orto-photos of 1:40,000 (1 m of resolution) available at Geographical Institute of Portugal were used for coastal line digitalisation.

The environmental assessment of the estuary is then performed firstly by the quantification of the *Driving forces* and *Pressures* indicators, of the DPSIR framework, in the terrestrial boundaries and in the estuarine water (Chapter 6) and secondly by the quantification of the indicators of *State* and *Impact* (Chapter 8, 9 and 11) in each management unit. Data that was not available in literature for the characterization of the management units needed still to be quantified. Only a set of indicators scored with higher feasibility and relevancy could be quantified in this stage. The overall quality assessment of the management units is assigned by the integration of these DPSIR categories (Chapter 11).

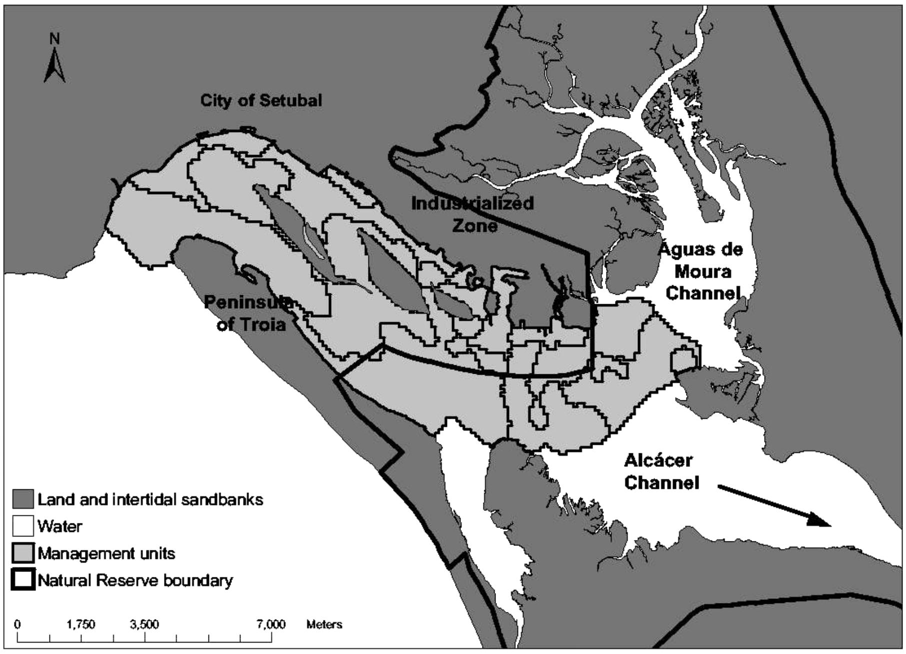

Figure. 2.3 – Sado Estuary management units within digitised coastal line. Natural Reserve boundary from Painho *et al.* (1996).

The Sado Estuary environmental management unit's diagnosis was developed by different exploratory analysis, namely aggregation of indicators into different indices, spatial analysis and statistical treatment, overlaying the indicators of the different categories of the DPSIR in a GIS platform.

This management tool could then be integrated with an ecological and dynamic model already developed for the estuary (used in HIDROMEDE, 1998 study). This integration with the EMMSado framework allows useful outputs within the management tool. The sediment transport model package helps, for instances, to calculate which estuary area will suffer an effect and resulting *Impact* due to a certain *Pressure* indicator. *Responses* action forecast will also be possible using an ecological and dynamic model package. These *Responses* measures will change the quantitative *Pressure* and resulting *State* and *Impact* (Painho *et al*., 2002 – see Annex II).

The integration between environmental and socio-economical data in the GIS will allow the construction of a management support tool easily used by end-users like the administration or Natural Reserve, local authorities or consulting private enterprises. This interface is based on a Sado Estuary Digital Atlas connected to an existing database with different thematic maps (namely, integrated environmental quality assessment; social and economical pressures, priorities operations of riparian/restoration). This management and planning tool is essential for the rehabilitation and recovery of the Sado Estuary zones already contaminated and for assuring conservation and biodiversity of protected areas.

2.5 CONCLUSIONS

The aim of this work was to describe an ongoing methodology for an environmental management system for Sado Estuary based on the application of DPSIR framework developed in a GIS. The DPSIR framework can be a useful and efficient tool for environmental data management namely when the data exists in a disperse and not synthesised way and where it is essential to apply environmental management measures, such is the case of Sado Estuary.

Based on Sado Estuary characterisation data and indicator concepts and criteria for their selection, the different indicators and/or indices belonging to the five categories of the DPSIR framewok were selected. The categories of the framewok are then quantified in management units previously defined. To evaluate the *State* and *Impact* of the Estuary particularly importance was given to the sediment and benthos compartments due to its behaviour of contaminant accumulation, reflecting average conditions of long periods. The implementation of this methodology was developed in GIS environment using the indicators and indices supported by the DPSIR model, which include the environmental, social and economical data. At the end of the on-going project a management support interface will be available to end-users. The data will also be available to the public in general, namely through a web site.

This methodology although applied in this study to Sado estuary, can be applied to any coastal zone and used for the assessment of environmental conditions, elaboration of management plans and design of specific restoration/conservation actions to be carried out by the responsible institutions.

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PART III

DELINEATION OF ESTUARINE MANAGEMENT UNITS

CHAPTER 3 – SPATIAL SAMPLING DESIGN FOR SEDIMENT QUALITY ASSESSMENT IN ESTUARIES

SPATIAL SAMPLING DESIGN FOR SEDIMENT QUALITY ASSESSMENT IN ESTUARIES

Caeiro, S., Goovaerts, P., Painho, M., Costa, M. H. and Sousa, S. (2003).
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ABSTRACT

Unusual difficulties are encountered when characterizing the spatial distribution of the properties that collectively define the state of estuaries. Owing to the variability of these estuarine conditions, greater sampling efforts are often necessary to describe estuarine environments, as compared to other aquatic systems. That is why in coastal management studies, where the collection of data is sometimes very difficult and time-consuming, a robust sampling strategy is essential. The aim of this study is to design a spatial sampling strategy for estuarine sediments, using prior information on the spatial variation of sediment granulometry. Systematic unaligned sampling with a grid cell size of 750 x 500 meters was chosen on the basis of semi-variogram analysis, and was shown to have distinct advantages. This design was sampled for sediment parameters using a Global Position System (GPS) receiver and mapped within the digitized shoreline of the estuary. The estuary shoreline was digitized on the basis of aerial ortho-photography with tidal ebb determination. The sampling is intended to define the boundaries of environmental management units (areas) for the Sado Estuary, situated on the west coast of Portugal. The research represents one of the initial phases in the development of a Sado Estuary environmental management system integrated into a Geographic Information System (GIS).

KEYWORDS: Geographic Information System, sampling design, estuaries, Arcview software, semivariograms, aerial photo digitalization.

3.1 INTRODUCTION

In estuaries large scale patterns of spatial variability include the longitudinal salinity gradient along the continuum between the estuarine drainage basin and the coastal ocean. Sources of small-scale spatial variability, unique to or amplified for estuaries, overlap this trend. These sources of small-scale spatial change include distributed point sources, such as human waste discharges; features of water circulation, such as fronts or convergences that create high local turbidity; or patchiness resulting from irregularities in bottom topography (Jassby *et al.*, 1997). Due to the variability of these estuarine conditions, greater sampling efforts are often necessary to describe estuarine environments, compared to other aquatic systems. That is why in coastal management studies, where the collection of data is sometimes very difficult and time-consuming, it is a prerequisite to design sampling strategies that detect the existing spatial heterogeneities (Kitsiou *et al.*, 2001). Sample size and design is also very important when the objective is to interpolate and create contour maps for a variable within a region (Haining, 1990).

Using a GPS-receiver for field sampling allows inclusion in a GIS for subsequent analytical, statistical and modelling analysis. The use of GIS technology for coastal management provides: i) great visualisation improvements of such data for space-use management; ii) enhanced use of remotely sensed data; iii) high quality graphical output for the dissemination of information; iv) development of efficient data and information management infrastructures (Ricketts, 1992) and v) combination of dissimilar data, such as socio-political boundaries, bottom types and habitat distributions (Stanbury & Starr, 1999). Remote sensing has shown itself to be cost-effective for mapping shoreline habitats when compared with land-based surveys (Mumby *et al.*, 1999). In particular, aerial photography has been used in a wide range of coastal applications. Its most extensive use has been for determining shoreline boundary variations. The integration of analytical GIS, GPS and remote sensing is an effective planning tool and a sound basis for continued coastal monitoring (O'Regan, 1996).

The aim of this study is to design a spatial sampling strategy for estuarine sediments, using prior information on the spatial variation. The design covers the small-scale variability and the uniformity of the study area. The sampling design strategy will be applied within an estuary boundary digitized from aerial ortho-photography. This sampling strategy is for the future definition of environmentally homogeneous sediment areas for the Sado Estuary, on the west coast of Portugal. This research represents one of the initial phases in the development of an environmental management system for the Sado Estuary, integrated into a GIS.

3.2 SPATIAL SAMPLING DESIGNS

The selection of a sample size and design, an estimator for the population characteristics and sampling variance are fundamental requirements for sampling experiments. The presence of spatial dependency has implications for all these stages (Haining, 1990).

As well studied in the literature, the three main forms of point sampling in a geographic region are simple random sampling, stratified sampling and systematic sampling. Spatial variables are almost always auto-correlated according to some scale, and in these circumstances simple random sampling is inefficient in the sense that it requires more effort to achieve a given precision than any other scheme. Stratified sampling is more precise than simple random sampling. In general, the smaller the cells, the smaller the within-stratum variance. Systematic sampling provides the most precise estimates for a given sampling effort (Cochran, 1977, Clark & Hosking, 1986, Haining, 1990, Thompson, 1992, Jassby *et al*, 1997, Webster, 1999).

For the local estimation of spatial variables, a regular grid is the most appropriate design (Flatman *et al.*, 1987 and Haining, 1990). Unfortunately, systematic sampling does not provide an entirely satisfactory assessment of the estimation variance because the sampling points are not randomized once the grid has been placed on the land. A potential hazard of systematic sampling is bias arising if a sampling grid is offset to one side or another of a region in which there is a trend in the variable of interest (Webster, 1999). In estuarine environments the abiotic and biotic variables are usually strongly dependent and vary according to the physical regimes of the estuaries, evaluated through the three main process agents: waves, tides and wind. One solution is to design a systematic unaligned sampling suggested by Berry and Baker (1968). The bias is reduced and the resulting design has greater precision than any of the other methods mentioned (Cochran, 1977). This approach avoids the periodicities of the systematic approach, gives good coverage over an area, is efficient, and deals with most distributions (Clark & Hosking, 1986).

The environmental monitoring and assessment program (EMAP) of the United States Environmental Protection Agency uses systematic sampling in areal coverage yet probabilistic sampling for its design (Overton *et al.*, 1990). In Delaware and Maryland Coastal Bays an appropriate number of EMAP grid cells is selected randomly for each subsystem of coastal bays and a random site from within theses cells is selected (Chaillou *et al.*, 1996).

Geostatistical approach for spatial sampling designs

A robust spatial sampling design applied to estuarine environments requires prior information on the spatial correlation in the estuary, which can be quantified using semi-variogram analysis (Burgess & Webster, 1984, Flatman *et al.*, 1987, Jassby *et al.*, 1997, Van Groenigen *et al.*, 1999, Van Groenigen *et al.*, 2000, Kitsiou *et al.*, 2001). Although highly successful in other areas, for example soils, few studies like for example Reed *et al.* (2000) have been conducted in estuarine environments using this kind of approach. The use of previous samples to direct additional sampling is important for the minimum kriging variance of regional variables (Van Groenigen *et al*, 1999).

The semivariogram $\hat{\gamma}(h)$ measures the dissimilarity between values of the regionalized variable z, $\{z(x_\alpha),\ \alpha = 1,\ldots\ldots, n\}$, with respect to the spatial separation h (Goovaerts, 1997):

$$\hat{\gamma}(h) = \frac{1}{2N(h)} \sum_{\alpha=1}^{N(h)} \left[z(x_\alpha) - z(x_\alpha + h)\right]^2 \qquad \text{(eq. 3.1)}$$

where $N(h)$ is the number of pairs of data locations a vector h apart. A model of spatial variability assumed to be characteristic of the sampled data is fitted to the experimental semi-variogram (Fig. 3.1). The semi-variogram reaches a plateau, c, at the range of correlation (a) since data separated by a larger distance are considered spatially independent. This distance is important for the sampling plan in that to collect non-redundant observations they must be at least a distance equal to the range of correlation apart. c_0 combines random variance factors, such as sampling and analytical error, along with any spatial variability that may exist at a distance smaller than the shortest sampling interval (Flatman *et al.*, 1987).

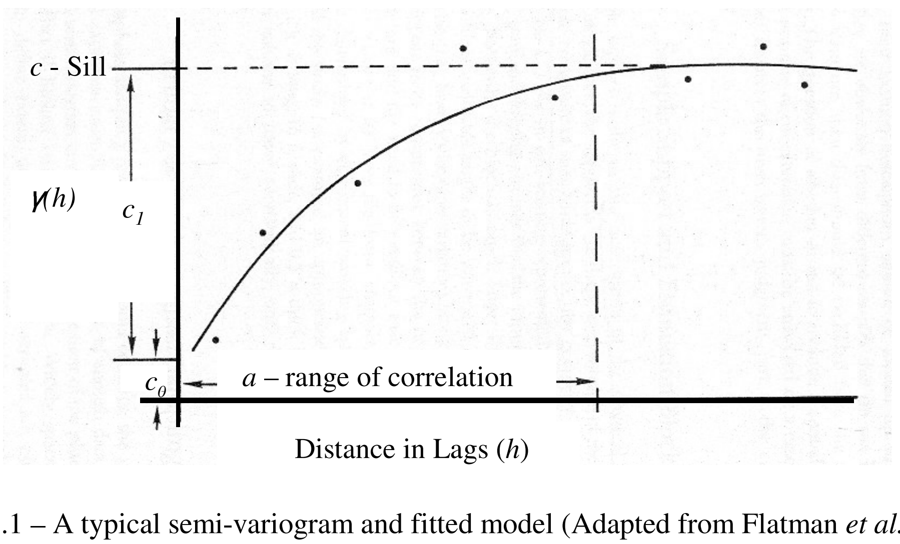

Figure 3.1 – A typical semi-variogram and fitted model (Adapted from Flatman *et al.*, 1987).

As already stressed, in estuarine environments the spatial variability is usually direction-dependent. Such spatial anisotropy is better identified when the experimental semivariogram values are plotted in the system of coordinates (h_x,h_y), yielding the semivariogram map (Goovaerts, 1997).

3.3 STUDY AREA

The Sado Estuary is the second largest estuary in Portugal, with an area of approximately 24,000 hectares. It is located on the west coast of Portugal, 45 km south of Lisbon, within a boundary box of 8º42' W 38º 25' N and 8º57' W 38º32' N. Most of the estuary is classified as a nature reserve. Exception is made for the city of Setúbal, its port, and a considerable part of its surrounding area. The Sado Estuary basin is subject to intensive land use practices and plays an important role in the local and national economy (Caeiro *et al*., 2002). The difficulties of the reserve authorities in managing urban growth and industrial pressures are also reflected in the higher urban growth rate inside the protected area boundary when compared with its surroundings (Painho *et al.*, 1999). This is probably due to the fact that numerous official bodies are responsible for land use planning in the reserve area, causing, at times, management bottlenecks.

3.4 METHODS

3.4.1 Coastal boundary digitization

Sado estuary coastal boundary was digitized on the basis of aerial ortho-photos of 1:40,000, 1m resolution (CNIG, 1995) using ArcView 3.2 ® (Image Analysis®) extension.

The estuary boundary was digitized using manual image classification (Robinson *et al.*, 1995). This feature extraction approach is a combination of manual interpretation and digital image display. Using the mouse, the polygon of the interpreted features was traced from the image displayed on the colour monitor. Polygons are drawn on the image as they are digitized and are also stored as a shapefile and included in a GIS database. This method is less time-consuming than digital image classification. The latter method uses image processing to classify each pixel, based on the reflectance value in each spectral band. Considering our objective, digital image classification produces complex polygons with delineation problems that are difficult to manage, require generalization and manual editing to remove errors (Fig. 3.2).

Sandbanks did not appear in aerial ortho-photo maps, owing to the height of the tide at the time the photos were taken. These morphologic structures suffer small changes in shape and location throughout time. However their continuous presence in the estuary has been observed during the recent decades. Theses structures were digitized using a 1:25,000 nautical chart (UKHO, 1999).

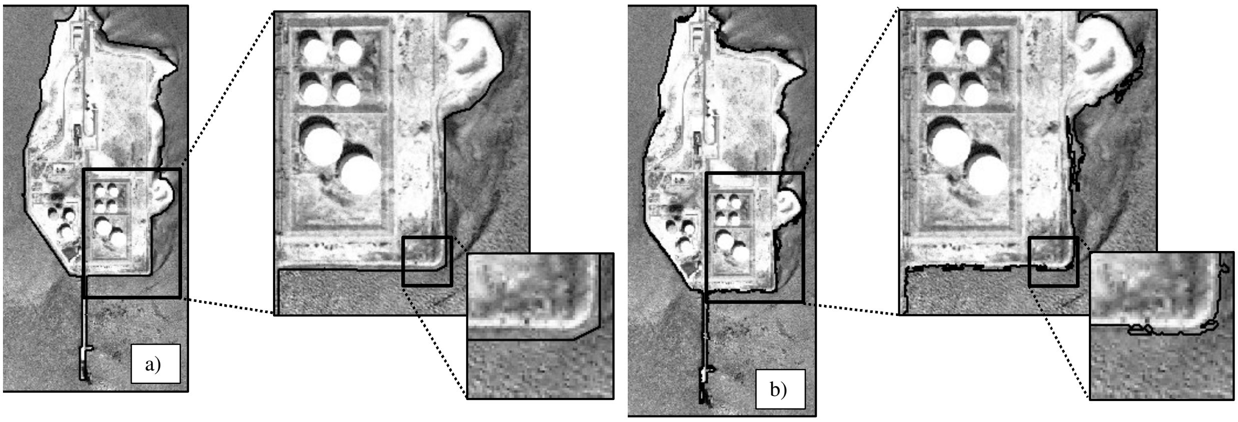

Figure 3.2 – Comparison between a) manual image classification and b) digital image classification.

The digital estuary boundary was mapped in the transverse Mercator projection, in Lisbon datum.

Since aerial photos were taken at different stages of the tide, digitized boundary gauging was needed. The height of the tide was calculated for each aerial photo, using the date and time of each photo and the tidal data for three local harbours (IH, 1995) (Fig. 3.3). The height of the tide at any time after low tide (y_1) was calculated with reference to an harmonic analysis of the marigraphic observation series of variable duration (IH, 1995):

$$y_1 = \frac{H_H + H_1}{2} + \frac{H_H - H_1}{2} cos\left(\frac{\pi t_1}{T_1}\right) \qquad \text{(eq. 3.2)}$$

where:
T_1 = the time lag between low tide and high tide (min) for each photo
t_1 = the time lag between low tide and the desired height of the tide (min)
H_1 and H_H = respectively, the height of the high and low tides that demarcate the desired time lag, in relation to mean sea-level (m).

The Thiessen method was applied to ascertain which ortho-photos were influenced by each piece of harbour tidal height data (H_l and H_H). Thiessen polygons, also referred to as the Dirichlet Tessellation or the Voronoi Diagram, define the individual ‘regions of influence’ around each of a set of points (Chrisman, 1997). This method does not take into account the estuary hydrodynamics, shape and channels. Since our study area was conducted in the estuary bay and not in highly convoluted short channels, this method provides a good estimation for linearly counted points.

3.4.2 Sampling design

A systematic unaligned design was chosen for sampling sediment characterization indicators to delineate environmentally management units in the Sado Estuary. Although systematic sampling is more suitable for interpolation, using random samples in each grid provides some clustered locations that can be very helpful to infer the semi-variograms at small lags.

Grid unit length was assessed through analysis of experimental semivariograms estimated using observations of a previous study (Rodrigues and Quintino, 1993). This work analysed sediment granulometry, a parameter strongly correlated with the sedimentary environment, at 133 sampling sites not regularly distributed along the estuary bay (see Fig. III.1 in Annex III).

According to Flatman *et al*. (1987), the distance between sample locations should be half the correlation range of experimental semivariograms (a/2) of previous data, in the case of a small nugget effect. In the case of a large nugget effect, sample distance should be less than two-thirds of the range of correlation (2a/3). The grid should be laid out with no vertices unsampled. Semivariograms were computed and modelled using the public-domain software Variowin 2.2.

3.5 RESULTS AND DISCUSSION

3.5.1 Coastal boundary digitization

The digitized boundary of the estuary is shown in Fig. 3.3. The computed average tide height differences between low tide and the tide at the time when the photos were taken was 2.52 ± 0.099 m, corresponding to 4 hrs 19 min ± 16 min, after the low spring tide. These tidal height differences are not relevant to our study area, because most of the shoreline is man made with a steep slope, and thus a small ebb area. The maximum difference between the height of the tide in the aerial photos (only 0.3 m) was minimized by choosing the lowest water level between two adjacent aerial photos for digitizing.

Despite the aforementioned limitations, this estuary boundary shows a satisfactory level of accuracy and validity when compared to other work, which has been carried out with other scales and sources of information (e.g. CNIG, 1990; Painho *et al.*, 1999; UKHO, 1999; Martins *et al.,* 2001). It is also the only known attempt to document an estuary line for this area. For the Troia Peninsula area (south of the estuary) Gomes *et al.* (2001) carried out a shore line evolution study from 1948 to 1997, using digitized photos and/on a scale of 1:40,000 to 1:2,000, though without taking into account tidal ebb variations.

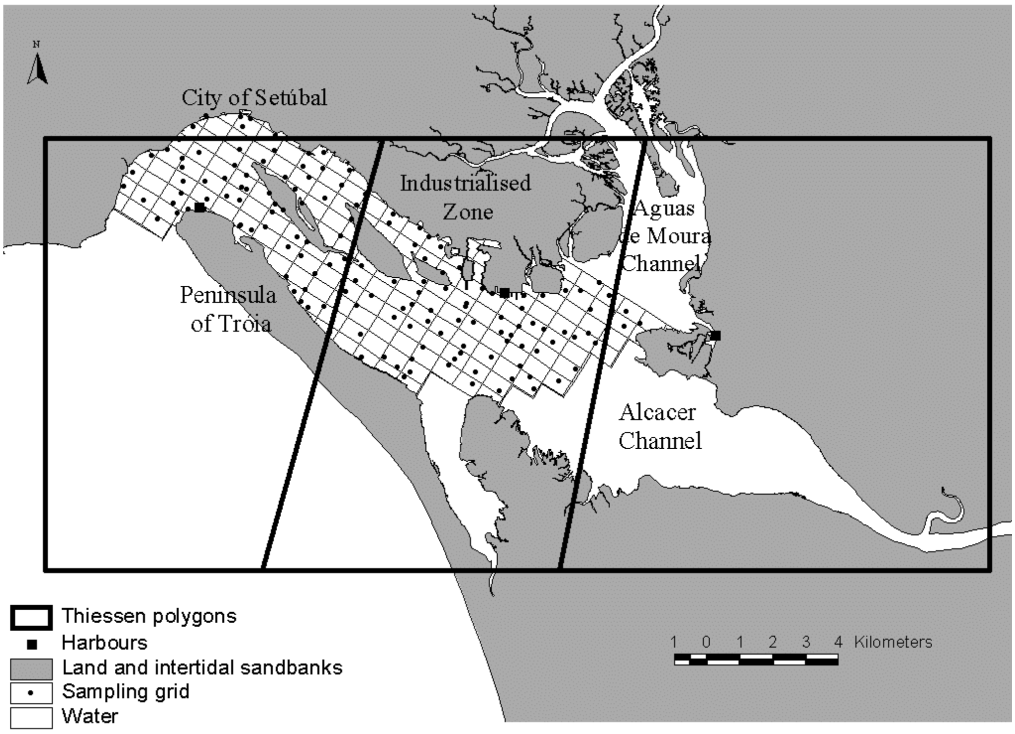

Figure 3.3 – Sado Estuary sediment sampling design within digitized boundary of the estuary.

3.5.2 Sampling strategy

The semi-variogram map (Fig. 3.4) of fine fraction particles shows a clear anisotropy, with the maximum continuity observed in the direction of azimuth 120º. This is due to the fact that the variability in the estuary bay is greatest in the direction perpendicular to the water flow, which is consistent with other studies (Martins *et al.*, 2001).

In the case of anisotropy a good strategy is to elongate the grid in the direction of the strongest correlation (maximum continuity) (Haining, 1990).

Few studies have computed semivariograms for estuarine sediment parameters like fine fraction contents. Reed *et al*. (2000) computed omnidirectional semivariograms for a particular sediment size of < 63 µm in a United Kingdom commercial dock and obtained a large nugget variance, with little spatial dependence. This latter fact shows anisotropy of the variability of fine fraction values. Without the comparison of semivariograms in at least two directions (major and minor spatial continuity) or ancillary information, like hydrodynamics, it is difficult to detect anisotropy and draw conclusions on spatial variability.

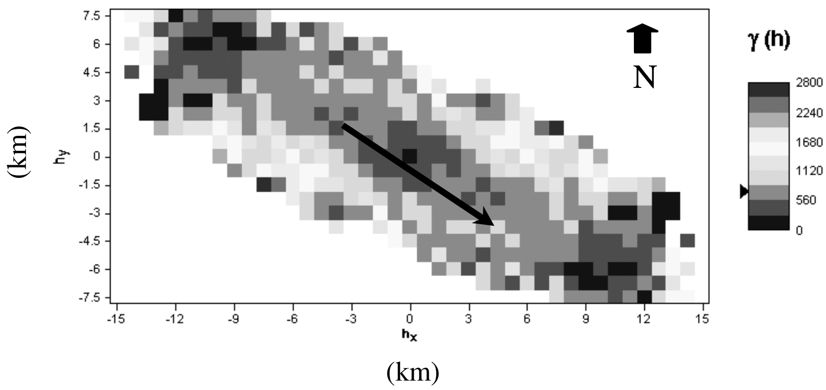

Figure 3.4 – Semivariogram map for fine fraction contents to detect anisotropy.

Semivariograms were computed up to a distance of 5 km in the directions of azimuth 30º and 120º (see Fig. 3.5). Lag distances of 0.25 km and angular tolerances of 30º were chosen since they yielded the most easily interpretable semivariograms. A spherical model with a range of 1.5 km in the direction of azimuth 120º and 1 km in the perpendicular direction was fitted. As a result, Fig. 3.3 depicts the final grid cell definition, extending 750 m in the direction of maximum continuity and 500 m in the perpendicular direction (*a*/2). A better explanation about the experimental semivariograms estimation and modeling fitting is available in Annex III.

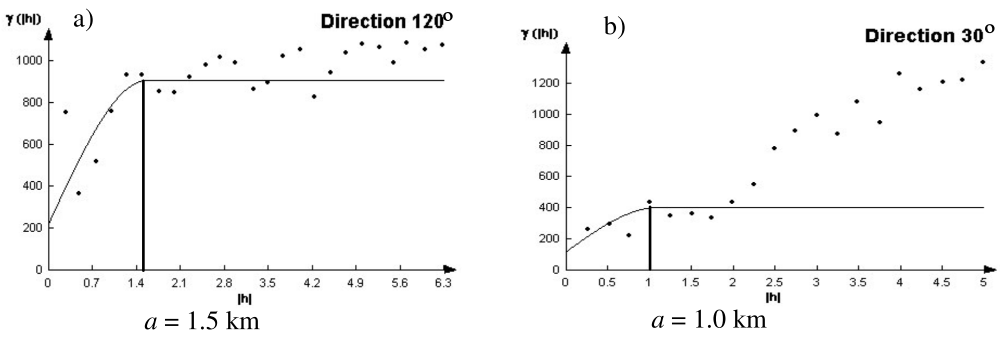

Figure 3.5 – Semivariograms for fine fraction percentages in the direction of maximum continuity (a) and in the perpendicular direction (b), with the spherical model fitted.

This design has already been successfully used for sediment parameter sampling. The final grid included 153 sites covering the estuary bay as far as the entry of the Águas de Moura and Alcácer Channels (Fig. 3.3) (sampling density of 153/57 km^2 or 2,68/ km^2). The random sampling point in each grid was attained every time the boat moved and reached a grid rectangle, using a GPS-receiver (Garmin GPS 12xL). This sampling was used for the further mapping of environmentally homogeneous sediment areas of the Sado Estuary applying geostatistical (i.e. kriging) interpolation techniques. Computed semivariograms of the fine fraction collected in this sampling campaign (Caeiro *et al*., 2003) confirmed the spatial variability previously calculated.

Most studies of sampling design for estuarine sediment quality are conducted without a statistical basis. The choice of sampling points is mainly based on local characteristics, like sources of pollution. It is only for national or regional estuarine monitoring programs with a reduced and representative number of samples that more careful statistical support is used (e.g. Overton *et al.*, 1990). Few studies have developed sampling strategy designs for the spatial assessment of coastal sediment quality (Table 3.1). The four studies listed in Table 3.1 show substantial differences in the density (from 0.018 to 135 locations per km^2) and spatial configuration of sampling points. These differences could be due to the spatial variability of sediment parameters in each coastal zone, in particular with the differences in geomorphological, biological and human pressures. These illustrate the importance of taking into account information from previous studies.

3.6 CONCLUSIONS

Statistical support including previous knowledge of spatial variability for sampling design definition is an essential preliminary step in ecological research. In spite of this, few efforts are being made to design sampling properly, in particular for spatial assessment of estuarine sediment quality. The aim of this study was to design a robust spatial sampling strategy for the Sado Estuary. Systematic unaligned sampling was chosen and its advantages discussed. A final grid of 750 x 500 m was then defined using prior information on the spatial variation in the estuarine sediments. Preliminary analysis of the sampled data collected shows valid and precise interpolation results for the definition of environmentally homogenous sediment areas in the Sado Estuary (Caeiro *et al*., 2003). This sampling was integrated into a GIS within a digitized Sado Estuary boundary, allowing future integration of environmental monitoring and management information. This boundary was digitized with the tidal knowledge acquired, which will also permit accurate studies of shoreline evolution and changes. These studies are of particular importance with regard to sea level changes related to natural or anthropogenic climate changes and any consequent variations in estuarine morphology.

Table 3.1 – Examples of spatial sampling designs in coastal sediment studies.

Coastal zone	Sampling design	Number of sites/area	Aim of the study	Author
Delaware Bay, USA	Stratified random sampling, according to EMAP	91/2059 km^2 (0.044/ km^2)	Assessment of the ecological conditions, including spatial distribution of sediment assessment	Chaillou *et al.* (1996) USEPA (1998)
San Diego Bay, USA	Direct sampling (for specific areas of concern) and stratified random (to identify spatial extent of regional toxicity)	350/35 km^2 (10/ km^2)	Spatial pattern assessment of sediment toxicity and chemical concentrations	Fairey *et al.* (1998)
Eastern waters of Hong Kong, China	Systematic grid of 5 km and transects running along the directions of local tidal movements	39/2079 km^2 (0.0188 km^2)	Interpolation (through Kriging) of contour map for sewage pollution	Poon *et al.*(2000)
King's Docks, Swansea, United Kingdom	Stratified sampling, grid of 405 m and additional sampling points located randomly from each grid node with a fixed range of distances between them of 135, 45, 15 and 5 m	101/0.75 km^2 (134.7/km^2)	Interpolation (through Kriging) of contour map and spatial scale of variation for PCB contaminant sediments	Reed *et al.* (2000)

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CHAPTER 4 – DELINEATION OF ESTUARINE MANAGEMENT AREAS USING MULTIVARIATE GEOSTATISTICS: THE CASE OF SADO ESTUARY

DELINEATION OF ESTUARINE MANAGEMENT AREAS USING MULTIVARIATE GEOSTATISTICS: THE CASE OF SADO ESTUARY

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ABSTRACT

The Sado Estuary is a coastal zone located in the south of Portugal where conflicts between conservation and development exist because of its location near industrialized urban zones and its designation as a Natural Reserve. The aim of this paper is to evaluate a set of multivariate geostatistical approaches to delineate spatially contiguous regions of sediment structure for Sado Estuary. These areas will be the supporting infrastructure of an environmental management system for this estuary. The boundaries of each homogenous area were derived from 3 sediment characterization attributes through 3 different approaches: 1) cluster analysis of dissimilarity matrix function of geographical separation followed by indicator kriging of the cluster data, 2) discriminant analysis of kriged values of the three sediment attributes, 3) combination of methods 1 and 2. Final maximum likelihood classification was integrated into a Geographical Information System (GIS). All methods generated fairly spatially contiguous management units (areas) that reproduce well the environment of the estuary. Map comparison techniques based on Kappa statistics showed that the resultant three maps are similar, supporting the choice of any of the methods as appropriate for management of the Sado Estuary. However results of method 1 seem to be in better agreement with estuary behavior, assessment of contamination sources and previous work conducted at this site.

KEYWORDS: Management units, multivariate geoestatistical tools, estuarine sediments.

4.1 INTRODUCTION

Coastal areas management is a critical, pressing issue, as these ecosystems are among the most endangered and sensitive environments in the world. The coincidence of high natural values and attractiveness for human use has led to conflicts between conservation and development. The Sado Estuary is a good example where these conflicts exist because of its location near industrialized urban zones and its designation as a Natural Reserve. Therefore, it has become quite inevitable to implement a model of environmental management based on methodologies that enable the evaluation of the Sado Estuary processes (Caeiro *et al.,* 2002). The delineation of fairly spatially contiguous regions can be very useful to simplify these ecosystems management models.

Spatial heterogeneity is a fundamental environmental characteristic and may therefore be associated with ecological information. The importance of the discontinuities between homogenous zones for the structure of the ecosystems and the ecosystem dynamics, as well as for the maintenance of ecological stability, has been well established (Kitsiou *et al*., 2001).

The use of boundary overlaps to measure spatial association is preferred to models (such as correlation and regression), which presuppose relationships among variables. Boundaries have inherent scientific interest because their locations reflect underlying biological, physical, and/or social processes. Nevertheless there is a need for true multivariate techniques where variance/covariance among the variables is explored and the contribution of each variable to the pooled metric is quantified (Jacquez *et al.,* 2000).

Geostatistical techniques like kriging allow estimation of attribute values at unsampled locations taking into account the spatial continuity of the data (Soares, 2000). Since kriging is preceded by an analysis of the spatial structure of the data, the averaged spatial variability of the data is already integrated into the estimation/interpolation process (Wackernagel, 1995).

Multivariate methods like principal component analysis, cluster analysis and discriminant analysis can be coupled with the different types of kriging (Oliver and Webster, 1989, Reed *et al.* 2000, Goovaerts, 2002) allowing one to group sampling sites that both have similar properties and are geographically close. With these multivariate geostatistical techniques interpolation is improved, small occurrences of one kind of land within others of fairly similar kind are disregarded and undesirable fragmentation avoided (Goovaerts 1997, Reed *et al.* 2000).

Some of these techniques have been successfully used in soil studies but few were applied to estuarine environments (Reed *et al*., 2000, Barabás *et al*., 2001) especially to estimate and map spatially contiguous areas for environmental management purpose.

The main purpose of this paper is to present and compare a set of multivariate geostatistical methodologies to define regions of sediment structure. These regions, described in this work as homogenous areas, are computed based on the subdivision of continuous sediment physicochemical properties. The technique is illustrated using the example of Sado Estuary management.

4.2 MATERIALS AND METHODS

4.2.1 Study area

The Sado Estuary is the second largest in Portugal with an area of approximately 24,000 ha. It is located in the West Coast of Portugal, within a boundary box of 8º42' W 38º 25' N and 8º57' W 38º32' N. Most of the estuary is classified as a Natural Reserve but also with an important role in the local and national economy. There are many industries mainly on the northern margin of the estuary. Furthermore the harbor-associated activities and the city of Setúbal along with the copper mines on the Sado watershed use the estuary for waste disposal purpose without suitable treatment. In other areas around the estuary intensive farming, mostly rice fields, is the main land use together with traditional salt-pans and increasingly intensive fish farms (Costa *et al.*, 1998, Cerejeira *et al.*, 1999, Caeiro *et al.*, 2002).

4.2.2 Sampling design

From November 2000 to January 2001, sediment samples were collected at 153 sites located using Global Positioning System (Garmin GPS 12xL)(Caeiro *et al.*, 2003 – see Chapter 3). A systematic unaligned sampling design was adopted to provide pairs of close observations required for modeling the short-scale variability as well as a uniform coverage of the area, which tends to reduce the average extrapolation error (Flatman *et al.,* 1987). The grid cells are 500×750 m, with their length aligned along the direction of azimuth 120º, which corresponds to the water flow and is expected to exhibit less variability (Martins *et al.*, 2001). The grid spacing was based on a preliminary study on the spatial distribution of sediment granulometry, a parameter strongly correlated with sedimentary environment.

4.2.3 Analytical procedures

At each location three replicates were taken with a *Petit Ponar* ® grab (6 in Scoopes 00890) and a composite sediment sample was formed. Three attributes, which are strongly related with composition and spatial distribution of benthic organisms as well as contaminant mobility/accumulation, were measured: fine fraction (FF) (%), redox potential (Eh) and total organic matter (TOM) (%). This set of sediment attributes integrates the most important properties that characterize the structure and behavior of the sedimentary environment. Also they are easy and fast to measure (Engle and Summers, 1998, Gibson *et al.*, 2000). Fine fraction was obtained by hydraulic separation, after organic matter destruction and disaggregation of particles (Buchanan, 1984). Redox potential was measured *in situ* using an electrode (Hanna Instruments model - H 13111). Total organic matter corresponds to the amount lost on ignition at 500±25 ºC for 4 hours.

4.2.4 Multivariate geostatistical analysis

Estuarine management units (areas) were delineated using three different approaches that combine geostatistical prediction and multivariate statistical analysis, see Fig. 4.1:

1. Cluster analysis of dissimilarity matrix that accounts for distances in both the attribute and geographical spaces, followed by indicator kriging of the classification.
2. Block kriging of the three attributes, followed by a discriminant analysis of K-means clustering predicted values.
3. A hybrid approach that combines the discriminant analysis of method 2 with indicator kriging used in method 1.

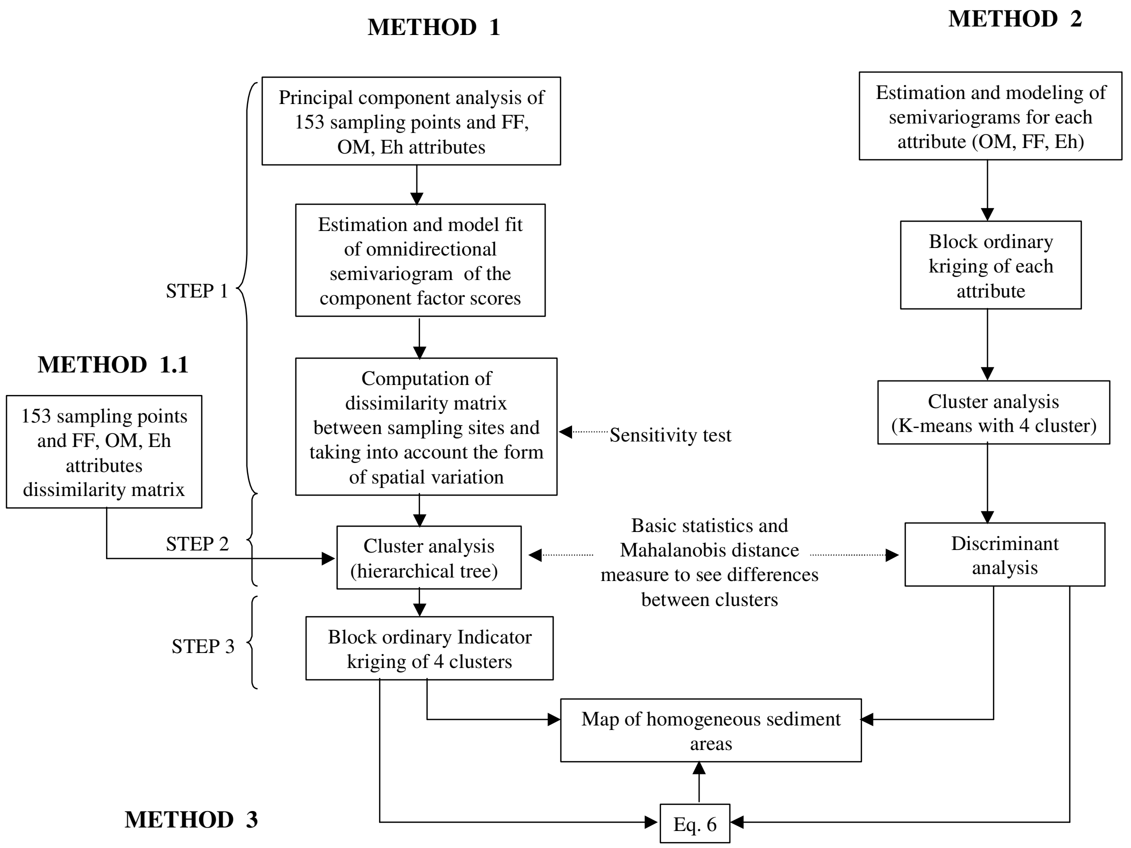

Figure 4.1 – Flowchart of the three methodologies used to delineate homogenous sediment areas.

Each approach yields, at each unsampled location (100 × 100 m grid), instead of a single class, a vector of probabilities of occurrence of the different categories or clusters. The final classification is obtained by maximum likelihood. Statistical analyses were conducted using Statistica 6.0 Software. Semivariograms were built in Variowin 2.2 and kriging was performed using WinGSLIB 1.3.1. The area corresponding to the sampling points was further clipped with the study area boundary including the coastline (Caeiro *et al.,* 2003 – see Chapter 3) using Arcview/arcinfo 3.2 GIS software.

Method 1

This method, described in Fig. 4.1, starts (Step 1) with a principal component analysis (PCA) of original data (FF, TOM and Eh), followed by computation of experimental semivariogram from the scores of a PCA and fitting of a spherical model. Following Oliver and Webster (1989) and with spherical model adjustment (Goovaerts, 1997) to take into account the form of spatial variation, the dissimilarity between any two sampling sites *i* and *j* is then computed as:

$$d_{ij}^{*} = d_{ij} \times \frac{c}{c_0 + c} \times \left[1.5 \times \frac{|u_{ij}|}{a} - 0.5 \times \left(\frac{|u_{ij}|}{a} \right)^3 \right] + d_{ij} \times \frac{c_0}{c_0 + c} \qquad \text{for } 0 < u_{ij} \le a$$

$$d_{ij}^{*} = d_{ij} \qquad \text{for } u_{ij} > a \qquad \text{(eq. 4.1)}$$

Where:

d_{ij} – distance in the attribute space between *i* and *j*

c - Sill of the spherical semivariogram model

c_0 - Nugget variance

a - Range of the spherical semivariogram model

u_{ij} - Euclidean geographic distance between *i* and *j*.

The measure d_{ij}^{*} tends to enhance the dissimilarity between sites that are geographically distant from one another. The use of semivariogram distance, instead of the Euclidian distance, allows one to account for the spatial variability inherent to the study site, in particular the possible existence of anisotropy (i.e. direction-dependent variability). In absence of any spatial correlation, the semivariogram value will be constant for any separation distance (pure nugget effect), and measure d_{ij}^{*} will identify the distance in the attribute space. The fitting of a model is necessary to be able to derive semivariogram value for all directions and classes of distances, even the ones that have not been sampled. PCA provides an easy way to summarize the information provided by multiple correlated attributes. Oliver and Webster (1989) and Reed *et al.,* (2000) found that the semivariogram of the leading principal components explained most of the spatially dependent variation, hence the semivariogram model of the first principal component is used in equation 4.1.

The Euclidean distance might become inappropriate as a measure of geographical separation if it relates to points over intervening land. Little *et al.* (1997), suggested the use of "in-water" distance computed as the length of the shortest in-water path between two sites, which requires contour maps and data layers for GIS analysis. Barabás *et al.* (2001) conducted a coordinate transformation prior to analysis, generating a grid within the river that "straightens out" the domain of analysis ensuring that distance are measured within the river. Because the present study is conducted in the estuary bay and not in highly convoluted and short channels, Euclidian distance provides a realistic measure of geographical separation.

In Step 2, d^*_{ij} values are assembled into a dissimilarity matrix that undergoes hierarchical clustering using the complete linkage rule (Everitt and Dunn, 2001).

In Step 3, indicator kriging is used to derive at unsampled locations the probability of occurrence of clusters identified in Step 2. The method starts with an indicator coding of classification results $Z(x_\alpha)$ at each sampled location x_α:

$$i(x_\alpha; z_l) = \begin{cases} 1 & \text{if } z(x_\alpha) = z_l \\ 0 & \text{otherwise} \end{cases} \quad l=1,\ldots,L \qquad \text{(eq. 4.2)}$$

where L is the number of clusters. For each cluster s_l, experimental indicator semivariograms are then computed and modeled:

$$\gamma(h, z_l) = \frac{1}{2N(h)} \sum_{\alpha=1}^{N(h)} \left[i(x_\alpha; z_l) - i(x_\alpha + h; z_l) \right]^2 \qquad \text{(eq. 4.3)}$$

Last, the probability of occurrence of the l-th cluster at the unsampled location x is estimated as a linear combination of indicator data:

$$\hat{p}(x; z_l \mid B_{geo}) = \sum_{\alpha=1}^{n_c} \lambda(x_\alpha; z_l) \times i(x_\alpha; z_l) \qquad \text{(eq. 4.4)}$$

Where B_{geo} is the set of n_c surrounding data $\{z(x_\alpha),\ \alpha=1,\ldots,\ n_c\}$. The weights $\lambda(x_\alpha;\ z_l)$ are solutions of an indicator kriging system and account for data configuration and spatial continuity of clusters as modeled by indicator semivariograms. Each grid node is assigned to the cluster with the highest probability of occurrence (maximum likelihood classification). Earlier works (e.g. Bierkens and Burrough, 1993, Goovaerts, 2002) already demonstrated the usefulness of indicator geostatistics as a methodology for modeling the spatial distribution of categorical variables and estimating probabilities of occurrence of classes based on surrounding observations.

In the end, this method generates relatively smooth maps showing locally dominant classes, uncluttered by outliers. This procedure fulfills the purpose of computing fairly contiguous sediment regions for management and monitoring purposes. To illustrate the benefits of this method, the resulting classification was compared to a map obtained when geographical distances are ignored (see Fig. 4.1 method 1.1 - unweighted geographical function).

Method 2

Unlike method 1, this technique first proceeds with the spatial interpolation of environmental attributes and then a clustering is computed to yield L clusters of sediment structure types. At the end discriminant analysis is used to compute the cluster classification probabilities at each unsampled location.

It starts with the computation and modeling of the 4 directional semivariograms of the three attributes (FF, TOM and Eh) (Fig. 4.1). Block ordinary kriging discretization by four points is then performed, yielding at each location x a vector of K=3 estimated attribute values, $B_w=\{\ w_k^*(x),\ k=1,\ldots,K\}$, allowing mapping smooth interpolation surfaces for each attribute.

A K-means clustering of 4 clusters was then performed on the block kriging entire set. A discriminant analysis is finally conducted with the K-means classification to compute the posterior probabilities of occurrence of each cluster at the unsampled locations. For the discriminant analysis each unsampled location will fall into one of the L clusters with the same prior probabilities of occurrence ($p_l = 1/L$). A tolerance value of 0.01 was used for each variable. Each grid node is then assigned to the cluster with the highest probability of occurrence, computed as:

$$p(x;\, z_l \mid B_w) = Prob\{Z(x) = z_l \mid B_w\} = \frac{p_l \times f(B_w \mid z_l)}{\sum_{l=1}^{L} p_l \times f(B_w \mid z_l)} \qquad l=1,\ldots,\, L \qquad \text{(eq. 4.5)}$$

where p_l is the prior probability of occurrence of class z_l at x, (i.e. $p_l = 1/L$ here) and $f(B_w|z_l)$ is the conditional density of attribute values W_k given the class z_l. The densities are estimated using a parametric method based on multivariate normal distribution theory (in this study the discriminant analysis was used).

Method 3

The main idea of this hybrid method is to find a way to account for local probabilities of occurrence of each group at unsampled locations, considering the spatial information, into the estimation of $p(x;\, z_l \mid B_w)$ of method 2. A simple approach is based on an equation developed by Goovaerts (2002) that computes the probability of occurrence of each cluster (l =1 to L) by replacing prior probabilities p_l in Bayes' expression (eq. 4.5) by IK-based probabilities (eq. 4.4):

$$p(x;\, z_l \mid B) = \frac{\hat{p}(x; z_l \mid B_{geo}) \times f(B_w \mid z_l)}{\sum_{l=1}^{L} \hat{p}(x; z_l \mid B_{geo}) \times f(B_w \mid z_l)} \qquad l=1,\ldots,L \qquad \text{(eq. 4.6)}$$

where the conditioning data set B includes both attribute (FF,TOM and Eh) and spatial information, $B=B_w \cup B_{geo}$. This approach amounts to assuming that the prior probability of occurrence of a class s_l is not the same everywhere, but depends on the location x. For example, the probability will be large if data belonging to cluster s_l are close geographically. A maximum likelihood classification is then performed on the vector of probabilities. Other works accounting for spatial coordinates (Goovaerts, 2002) have shown increases in overall accuracy. In reference Goovaerts, (2002) and in the present study, the same field data were used to derive the local probabilities of occurrence $\hat{p}(x; z_l \mid B_{geo})$ and the functions $f(B_w|z_l)$, although indicator kriging accounts for more information than the discriminant analysis that ignores spatial coordinates. This approach is however purely general and, for example, a training set from another region with similar characteristics could be used to derive the discriminant functions. Similarly the local probabilities of occurrence could be estimated from both field data and secondary information which might not be exhaustively sampled using a multivariate geostatistical approach.

Several statistics to compare the methods were computed, including Kappa index of agreement for categorical data. This statistic was adopted by the remote sensing community to assess map similarity and was computed following Cohen (1960).

4.3 RESULTS AND DISCUSSION

Distributions of fine fraction and organic matter are positively skewed, and natural logarithms were applied to make the distribution more symmetric and to stabilize the variance (Fig. 4.2 and Table IV.1 in Annex IV). Eh needed no transformation. The three variables are moderately correlated, suggesting that PCA would allow one to summarize this information.

In method 1, PCA was performed on the variance-covariance matrix of the three attributes, leading to a first principal component explaining 88 % of the total variance. Fig. 4.3 shows the corresponding semivariogram with the model fitted, which will be used for the computation of dissimilarity measures d_{ij}^{*} (eq. 4.1). The hierarchical classification yielded four clusters that are reasonably distinct, with a decline in organic load from Cluster 1 to 4, confirmed by an increase of the Mahalanobis distance between these clusters (Table 4.1, and Table IV.2 and fig. IV.1 in Annex IV). For each cluster, the indicator semivariogram was computed along four directions (Fig. 4.4 and Table IV.3 in Annex IV) and a geometric anisotropy model was fitted visually. All semivariograms display longer ranges in the direction of azimuth 120º, which corresponds to the water flow and is in agreement with other studies (Martins *et al.,* 2001). Fig. 4.5 (top graphs – methods 1 and 1.1) shows the results of the maximum likelihood classification performed on estimated probabilities, weighting and unweighting the geographical function. Clusters computed with the weighted geographical function show reasonable spatial continuity with, for a separation distance of up to 400 m, 50 % of locations belonging to the same cluster. This proportion is only 30 % if the cluster analysis is based on the dissimilarity measure d_{ij}, which ignores spatial coordinates of observations (see cluster in Fig. IV.2 in Annex IV), instead of d_{ij}^{*} (following Goovaerts and Webster, 1994 procedure - see Supporting Information and Fig. IV.3 in Annex IV). This hierarchical classification based on d_{ij}, also yielded a small cluster (cluster 3) of only 4 locations, distant from each other. It is not possible to classify this cluster due to the high standard deviations of the attribute concentrations (see Table 4.1 and Fig. 4.5– undefined group in method 1.1).

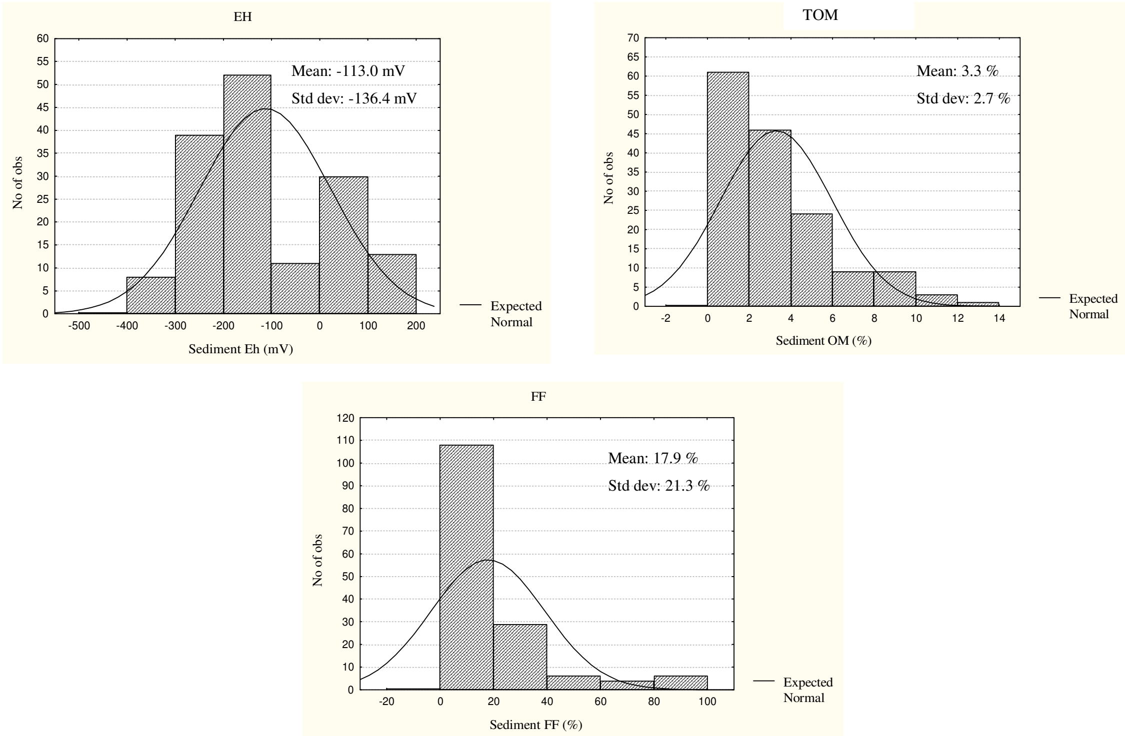

Figure 4.2 – Histograms and expected normal distributions of sediment redox potential, organic matter and fine fraction.

The unweighted classification of method 1.1 apparently created a reduced number of areas, since it classifies the major part of the estuary as Medium High organic load (65 %, due to a large area occupying 36 km^2 of the estuary – see Table 4.1), followed by low organic load classification (23 %). This classification does not reproduce the estuary behavior as explained further in this work. Also it creates a high percentage of areas smaller than the grid cell size ($\leq$ 0.375 km^2) (74 % of the total nº of areas). All these reasons support the use of multivariate geostatistics in method 1, as a tool for delineation of estuarine management units. Method 1.1 was thus discarded for further use.

Method 2 started with the computation of experimental semivariograms for each attribute (FF, TOM and Eh) and the fitting of an anisotropic model (Fig. 4.6, and Table IV.4 in Annex IV)[•]. The discriminant analysis with the calibration of 4 K-mean clusters predicted values, yielded a total of 97.5 % correctly classified locations. The organic load in the discriminated clusters decrease from cluster 1 to 4, as illustrated by an increase in the Mahalanobis distance between them (Table 4.1 and Table IV.5 in Annex IV). The resulting homogenous areas of Sado estuary are depicted in Fig. 4.5.

[•] Cross-validation procedures were computed to evaluate the impact of the semivariogram models on interpolation results (see Annex IV).

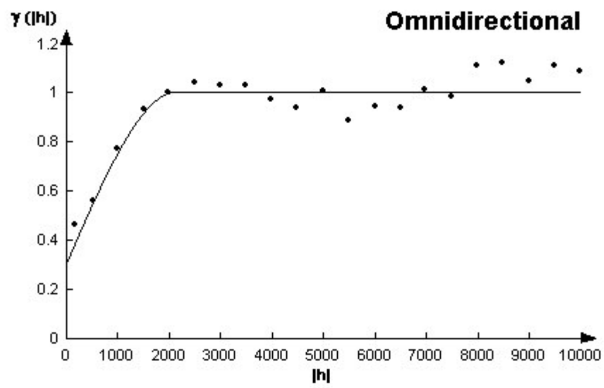

Figure 4.3 – Experimental semivariogram of the first principal component with the spherical model fitted. c_0 = 0.31; a = 2159 meters and c= 0.7.

In method 3, the homogenous areas were delineated by combining the previous two methodologies using eq. (4.6) (Fig. 4.5).

Table 4.1 – Statistics regarding the number and area of patches produced by the four classification approaches. LO – Low Organic load; MO – Medium Organic load; MHO – Medium High Organic load; HO – High Organic load; Und- Undefined.

Method	Groups	TOM (%)	%FF (%)	Eh (%)	Total area (%)	Nº of areas	Minimum area (km^2)	Maximum area (km^2)
1	1. HO	8.6±2.4	60.4±27.0	-278.9±68.6	9.48	19	0.0005150	1.06
	2. MHO	4.2±1.4	21.7±11.8	-178.8±72.6	38.24	26	0.0000110	9.13
	3. MO	1.9±0.7	9.1±7.8	-137.4±50.9	28.15	13	0.0014370	6.28
	4. LO	0.9± 0.3	1.5±1.3	74.4±49.0	24.11	12	0.0000100	8.00
				Total number of areas	70			
				Number of areas ≤ 0.375 km^2	51			
1.1	1. HO	7.6±2.4	50.5±25.7	-245.7±80.3	11.70	15	0.0087419	1.45
	2. MHO	2.9±1.3	14.1±9.3	-171.8±56.0	65.12	11	0.0000008	35.96
	3. Und.	5.3±1.6	34.0±20.2	11.1±53.7	0.28	4	0.0300000	0.05
	4. LO	0.9±0.4	1.7±1.9	74.4±48.4	22.91	8	0.0300000	7.49
				Total number of areas	38			
				Number of areas ≤ 0.375 km^2	28			
2	1. HO	4.1±0.9	23.2±9.1	-237.9±41.0	21.58	17	0.0000008	2.93
	2. MHO	2.9 ±0.4	13.0±3.9	-152.1±41.6	34.58	17	0.0005310	6.27
	3. MO	1.9±0.3	6.1±2.4	-78.7±52.3	28.15	7	0.0010410	13.68
	4. LO	1.1± 0.2	1.5 ± 0.7	45.4±47.1	15.71	7	0.0300000	6.66
				Total number of areas	48			
				Number of areas ≤ 0.375 km^2	29			
3	1. HO	same as method 2			16.02	22	0.0000013	1.97
	2.MHO	same as method 2			40.75	15	0.0008560	9.93
	3. MO	same as method 2			25.98	15	0.0010410	11.20
	4. LO	same as method 2			17.24	8	0.0100000	7.09
				Total number of areas	60			
				Number of areas ≤ 0.375 km^2	41			

Despite some differences between methods 1, 2 and 3 (see Table 4.1) their results generally are in agreement with earlier work performed in the estuary (Rodrigues and Quintino, 1993).

Low organic load sediments correspond essentially to the estuarine entrance and tend to extend to the inside of the estuary, basically through the southern channel. This is confirmed in all method results by the presence, at the estuary entrance, of a large homogenous area of low organic load (Fig. 4.5).

At the middle of the estuary bay the gradient splits into two major components, one directed towards the North Channel and the other towards the South Channel. All methods indicate that in the estuary bay the class of medium high organic load is of largest extent (until 40 % of the total area - Fig. 4.5 and Table 4.1). Since high organic load areas are associated with low hydrodynamics and rich organic discharges, they are more common in the North Channel near industrialized zones and the city of Setúbal. They are also distributed in small homogenous areas (Fig. 4.5). In methods 1 and 3, those areas are the less important in the estuary bay, representing respectively 9.48 and 16.02 % of the total study area (Table 4.1), while the proportion is 21.58 % for method 2 (Fig. 4.5 and Table 4.1). According to historical and expert knowledge of the estuary, this last proportion is an overestimation of this type of sediment. However, special care must be taken when comparing high organic load clusters for methods 1, and 2 and 3. High organic load cluster of methods 2 and 3 displays smaller values for TOM and FF and higher values of Eh. Method 2 produced a smaller total number of areas (48, comparing to 70 and 60 in methods 1 and 3, respectively), and fewer areas smaller than the grid cell size (Table 4.1).

Stratifications produced by methods 2 and 3 share similar spatial patterns (Fig. 4.5). Analysis of the Kappa values shows almost perfect agreement between Maps 2 and 3 (Kappa = 0.85) (Sousa *et al.* 2002 – See Chapter 5 and Annex V.1). This result might be due to method 3 be a refinement of the discriminant analysis applied in method 2 using the local probabilities estimated with indicator kriging in method 1. The main differences reside in smaller areas of high organic load and larger areas with medium high organic load in method 3 (Table 4.1 and Fig. 4.5). The spatial contiguity of the interpolated clusters of method 2, combined with the high density and systematic sampling of sediment, can explain the lack of benefit of using the indicator kriging probabilities in method 3.

Method 3 is moderately similar to method 1 (Kappa = 0.55). These maps are created using different multivariate geostatistics but method 3 uses results from method 1.

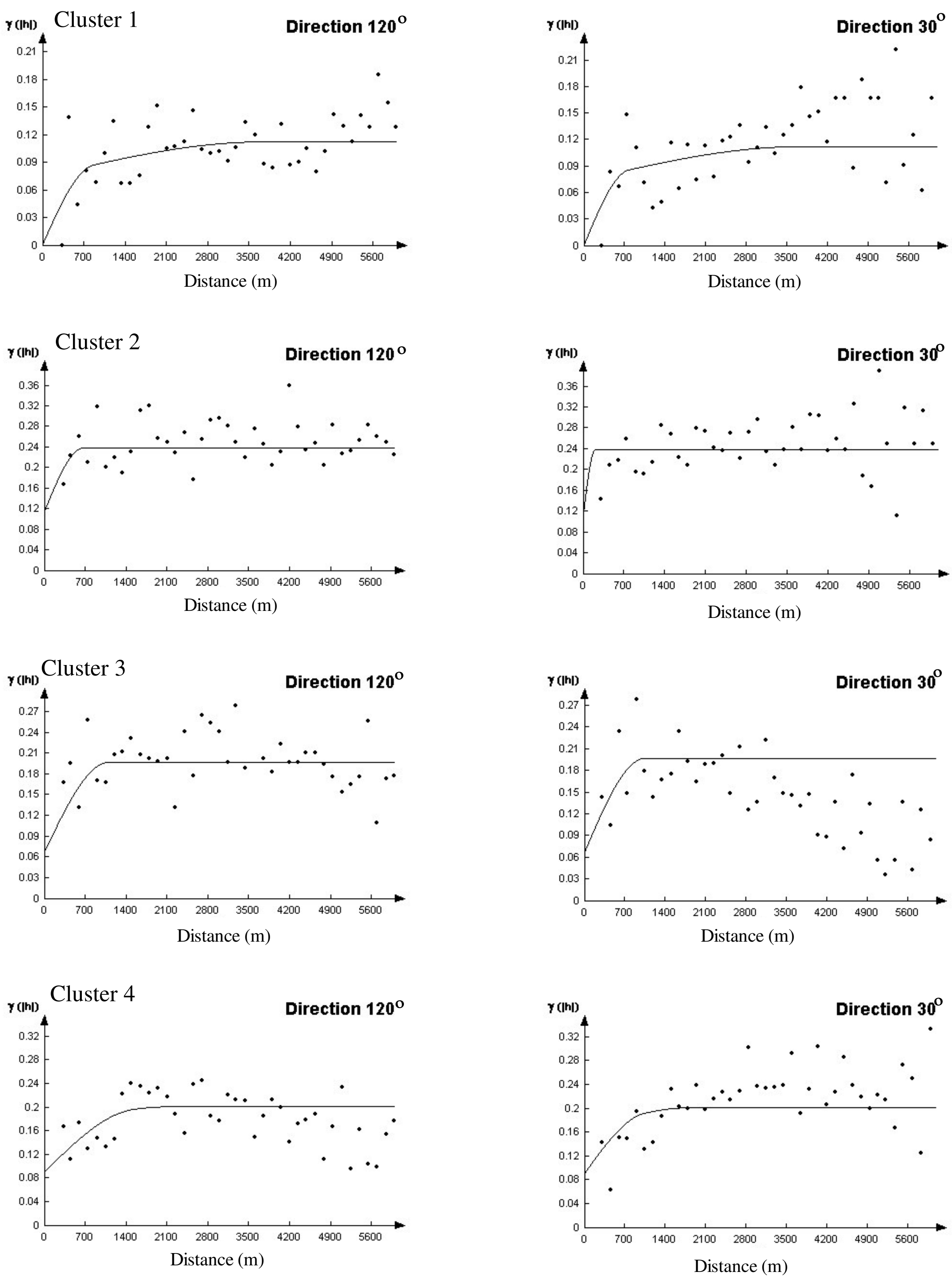

Figure 4.4 – Experimental directional semivariograms of cluster data, with the model fitted for 120º, the major direction of anisotropy, and the perpendicular direction, 30º.

Methods 1 and 2 are the ones with less agreement (Kappa = 0.42) since the computed management units use independent interpolation techniques (Sousa *et al*. 2002 – See Annex V.1).

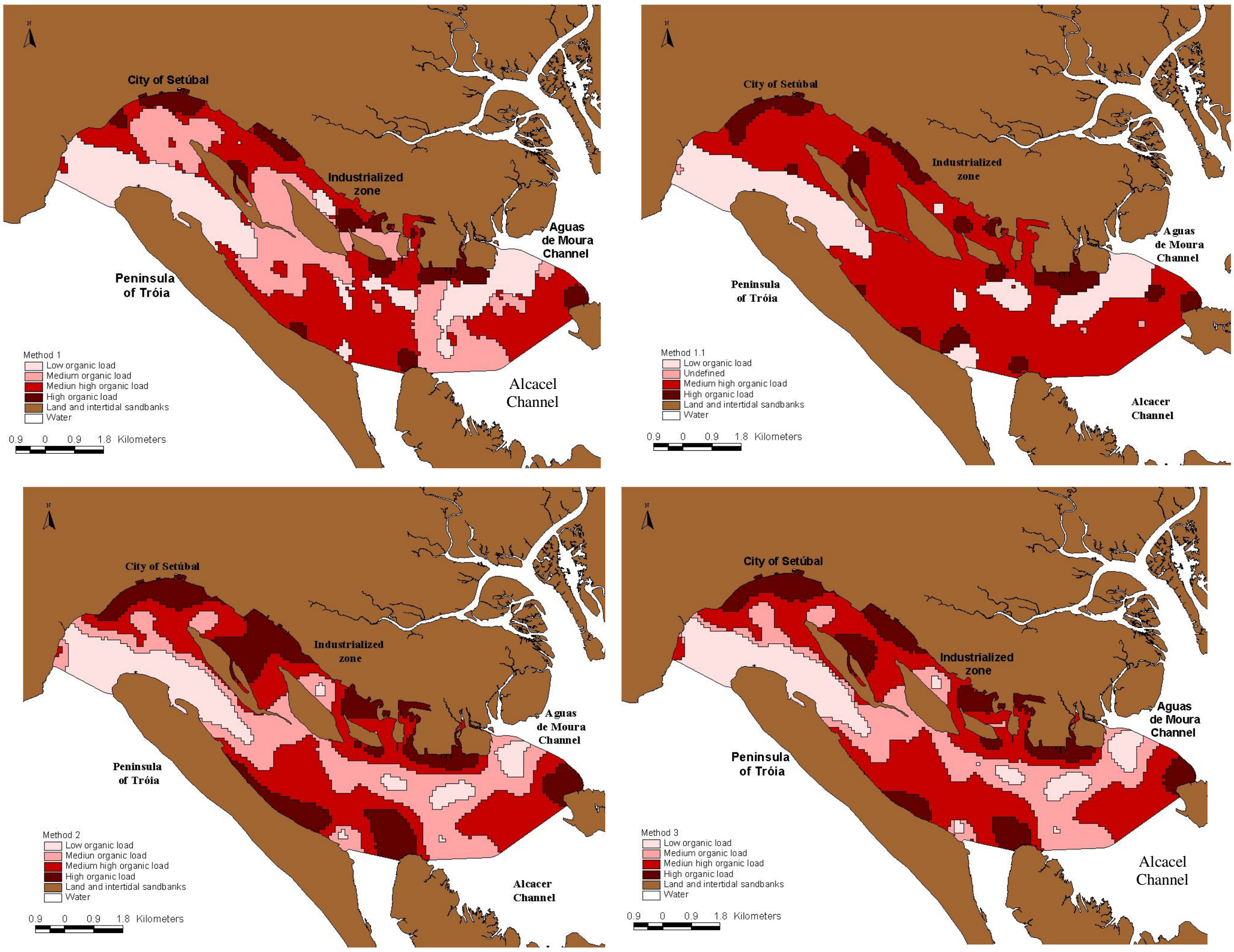

Figure 4.5 – Homogenous management units for Sado Estuary generated by methods 1 to 3.

The higher number of areas smaller than the sampling grid size (see Table 4.1) is also due to the clip with the study area boundary and should be ignored for delineation of estuarine management units. It was only considered important in this paper for the original methods comparison. In further developments of this large project of estuarine management, areas smaller than the sampling grid size are assigned to the neighboring area that shares the longest common boundary (Caeiro *et al.* 2004 – see Chapter 7).

4.4 CONCLUSIONS

In conclusion, after discarding the smallest areas, all methods will yield 19 management units (Table 4.1) that are fairly contiguous and reproduce well the estuary environment. Also the Kappa values indicate that the maps are similar, according to Landis & Koch (1977) classification, supporting the choice of any of the methods as appropriate for management of the Sado Estuary. Nevertheless method 1 seems to be in better agreement with estuary behavior and earlier work conducted in the estuary in terms of estuary hydrodynamics (Martin *et al.,* 2001), spatial distribution of sediment structure and benthic faunal assemblages (Rodrigues and Quintino, 1993), and identification of areas of contaminant sources. In summary method 1 shows a more realistic pattern and detection of focal areas important for cost-effective management and thus long-term monitoring.

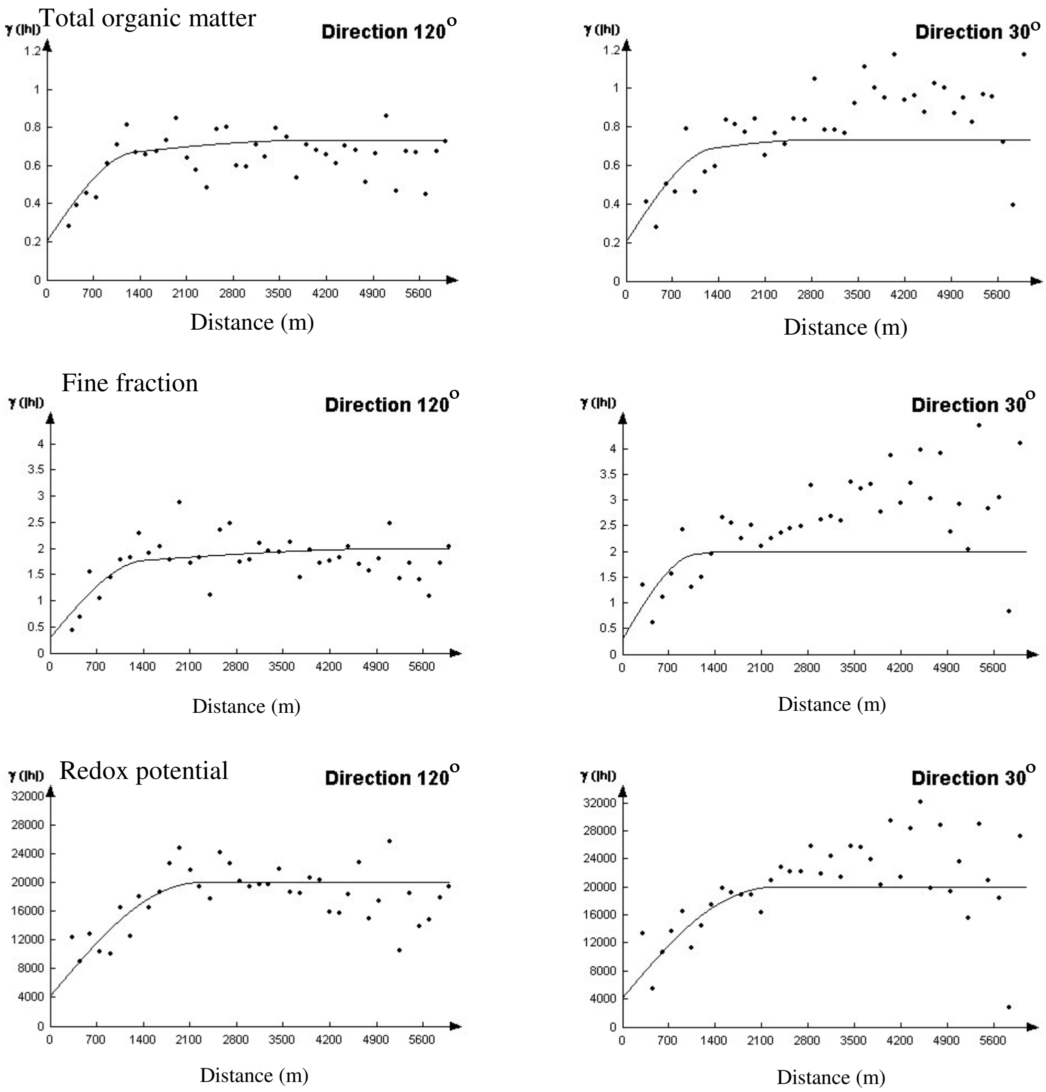

Figure 4.6 – Experimental directional semivariograms and model fitted in the major and minor directions of anisotropy for the three attributes.

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CHAPTER 5 – MAP SIMILARITY MEASUREMENT AND ITS APPLICATION TO THE SADO ESTUARY

MAP SIMILARITY MEASUREMENT AND ITS APPLICATION TO THE SADO ESTUARY

Caeiro, S., Sousa, S., Painho, M. (2003)

Finisterra **75** (*in press*)

ABSTRACT

In the past thirty years GIS technology has progressed from computer mapping to spatial database management, and more recently, to quantitative map analysis and modeling. However, most applications still rely on visual analysis for determining similarity within and among maps. The aim of this study is to compare maps of homogenous areas computed from estuarine sediment characterization indicators, using different approaches. These maps were defined using three different interpolation methods. Different Kappa statistics, visual map overlays or components of agreement and disagreement owing to chance, quantity and location were used for single cell and/or neighborhood (hard and soft) map comparison. Although the three methods were computed with different statistical techniques, their results are similar, supporting the choice of any of the methods as equivalent and thus of equal value to be used as management units of the estuary. Hence the significance of choosing one of the methods is reduced.

KEYWORDS: categorical maps, binary comparison, Kappa statistics, neighborhood statistics, estuarine management.

5.1 INTRODUCTION

In the different Geographical Information Systems (GIS) applications, the environment in general and costal areas in particular, comparing or detecting different categorical maps is an essential issue. The accuracy of a comparison procedure based on a more reliable and robust approach could lead to a marked improvement in the ability to detect a map change.

The simplest way to compare two maps is to compute the correlation between the mapped variables. But with this method the locations of the points are not considered. This reflects a major drawback on the method in an overall comparison, because a given correlation may reflect the degree of correspondence over the entire map area, or may be the result of a large deviation in a small region of the map (Davis, 1986). Map spatial comparison procedures are then, amongst others, important for the validation and calibration of spatial models (Hagen, 2002b). These procedures can express the similarity between two maps by looking at simple proportions of areas or by measuring it numerically. This numerical similarity can be assessed by categorical representation of overlay results as a contingency table. Statistical analyses are then made with various integral measures of association, log-linear models, among others (Zaslavski, 1995). When the assessment consists of a number of pair-wise comparisons, based on a cell-by cell agreement using the confusion matrix, the Kappa statistic (Cohen, 1960) can be a suitable approach (Carletta, 1996). The result of a map comparison can be an overall value for similarity (e.g. a value between 0 and 1) or a map in its own right, which means that the result of a comparison of two maps is a third map indicating per location how strong the similarity is (Hagen, 2002b). However the confusion matrix fails to distinguish between a near miss and a far miss maps. In other words, the confusion matrix records zero agreement when a cell is not classified correctly, even when the correct category is found in the neighboring cell, or even when the correct category is found nowhere near the cell (Pontius, 2002, Pontius and Suedmeyer, 2004).

There is wide disagreement about the usefulness of Kappa statistics to assess rater agreement. The model for chance agreement is statistical independence, which is not the expected basis within or between coverages (Chrisman, 1997). Kappa statistics should not be viewed as the unequivocal standard or default way to quantify agreement and alternatives to make an informed choice should be considered. Nevertheless it has easy calculation and appropriateness for testing whether agreement exceeds chance levels for binary and nominal ratings (Uebersax, 2003). Also new variants of Kappa were recently introduced to consider similarity of location (Pontius, 2000) and quantity (Hagen, 2002b).

When the comparison is to be made in non-static environments, like coastal environments it is difficult to define sampling grids in exact positions and therefore a single cell-by-cell analysis comparison is less representative If a specific cell fails to have the correct category, then it is counted as complete error, even when the correct category is found in a neighboring cell. Cell-by-cell analysis can fall to indicate general agreement of pattern because it fails to consider spatial proximity to agreement (Pointius and Suedmeyer, 2004). Therefore, in this case, a neighborhood cell comparison is more appropriate. Using the neighborhood to compare categorical maps could be computed using a hard or soft classification.

Neighborhood hard statistics using a mode function are very similar to frequency filters. These filters count the frequency of the attribute values occurring in a chosen window with a fixed size. The majority filter selects the value with the highest frequency. Majority filters are very useful for smoothing irregular edges between adjacent areas and they eliminate rare attribute values from a raster (Molenaar, 1998). A wide variety of functions can be used for hard neighborhood calculations depending on the goal of the work, but Mode is the more accurate for categorical data (Murteira and Black, 1983). Hard neighborhood operations summarize the attributes occurring in the vicinity of each location. It creates a new map where the value assigned to a location is computed as a function of independent values surrounding that location. This group of operations can be conceptualized as "moving windows" sliding throughout the mapped area.

However hard classification has the disadvantage of modifying the maps before the comparison. After hardening, there could be a substantial change in the quantity of each category, leading to errors and misleading results. By applying soft classification (also called further on this work fuzzy) for the comparison of categorical maps it is possible to obtain a spatial and gradual analysis of the similarity of two maps at different multi-resolution. In addition, it would be helpful to have on that soft comparison an analytical technique that allocates the sources of agreement and disagreement indicating in what respects the comparison map is strong and weak (Pontius and Suedmeyer, 2004).

Within GIS usually the map comparison statistics are used mainly for remote sensing, measuring the goodness-of-fit of simulation land-change models (e.g. Pontius, 2000, Pontius and Schneider, 2001, Hagen, 2002a) b) and c), and Pontius, 2002) and not to evaluate differences between spatial patterns models of regions with very dynamic characteristics like estuaries.

The team has been working on the development of an environmental data management system through sediment quality assessment for the Sado Estuary (EMMSado) in the south east of Portugal (Caeiro *et al*., 2002 – see Chapter 2) (Fig. 5.1). The units of this management system are spatially contiguous regions of sediment structure (homogenous areas). To delineate these management units three maps were computed using different multivariate geostatistical approaches. A great agreement of similarities will further support the choice of any of the methods as equivalent, and hence the less significance of choosing one of the methods.

The aim of this work is to assess the difference between the three maps using different similarity assessment approaches: 1st approach: single cell comparison using binary comparison and Kappa standard and its new variants Klocation to evaluate agreement due location and Khisto to evaluate agreement due to quantity; 2nd approach: hard neighborhood comparison, using binary comparison and Kappa statistic; 3rd soft neighborhood comparison using components of agreement and disagreement due to change, quantity and location. The advantages and disadvantages of using these different approaches are also compared and discussed.

5.2. METHODS

5.2.1 Previous work

The three Maps of management units were computed based on three sediment characterization indicators (fine fraction, organic mater and redox potential), using:

Method 1: Cluster analysis of dissimilarity matrix that accounts for distances in both the attribute and geographical spaces, followed by indicator kriging of the classification (Map 1).

Method 2: Block kriging of the three sediment indicators, followed by a discriminant analysis of K-means clustering predicted values (Map 2).

Method 3: A hybrid approach that incorporates the probabilities of occurrence at unsample locations of indicator kriging used in method 1 into discriminant analysis of method 2 (Map 3). (Caeiro *et al.,* 2003a – Chapter 4) (Fig. 5.2).

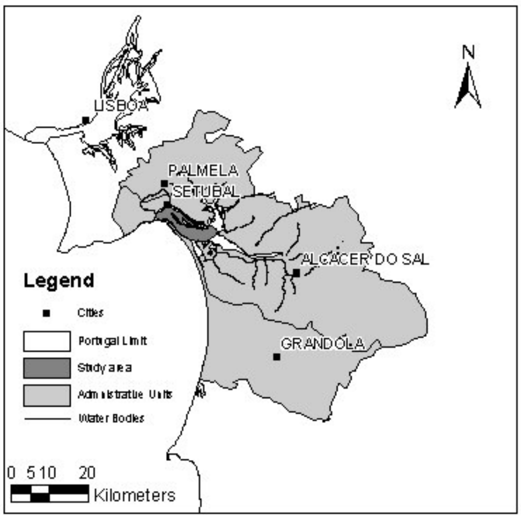

Figure 5.1 – Study area in Sado Estuary.

These interpolations were based on a systematic unaligned sampling campaign in 153 points spread over a final grid of 750 x 500 m, using prior information on the spatial variation in the estuarine sediments (CAEIRO *et al.*, 2003b – see Chapter 3). In each of these categorical maps, four organic matter contents categories were computed: 1- High, 2- Medium High, 3- Medium, and 4- Low Organic Load. Results of Map 1 seem to be in better agreement with estuary behavior, assessment of contamination sources and previous work conducted at this site (Caeiro *et al.*, 2003a - see Chapter 4). For that reason, Map 1 was considered the reference for the comparison between Map 1 and Map 2 and Map 1 and 3. For comparison between Map 2 and 3, Map 2 was considered the reference since Map 3 results are from a refinement of Map 2 using data from Map 1.

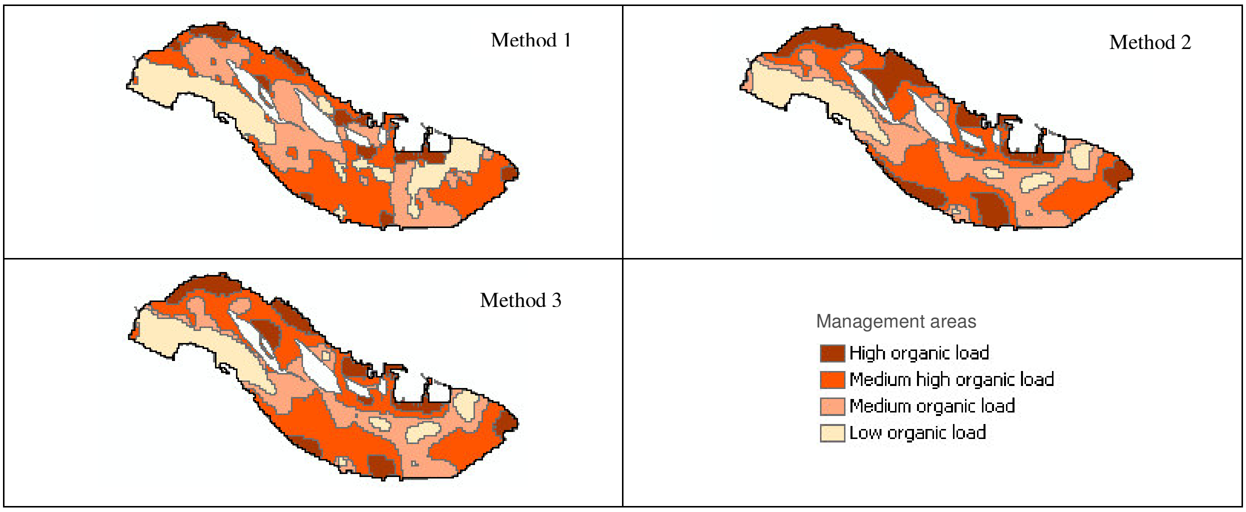

Figure 5.2 – Maps representing the 3 methods for Sado estuary management area delineation.

5.2.2 Single cell comparison

This first comparison approach involved the overlay of the original maps on a cell-by-cell basis, to produce a map and attribute table of site specific differences. Simple map algebra operations (union) were used. Then, based on the contingency table (or confusion matrix), Kappa and variants were calculated. Klocation, as discussed by Pontius (2002), was used to access the similarity of location, and Khisto, as developed by Hagen (2002b), was used to access the similarity of quantity (Fig. 5.3). These Kappa calculations are explained in a previous work (Sousa *et al.*, 2002 – see Annex V.1). Binary classification was computed using raster calculator and reclassify within ArcGIS^{TM} Spatial Analyst which states for each cell whether or not the maps are identical on that location.

5.2.3 Hard neighborhood comparison

In this approach each location is a function of the input cells of different neighborhood sizes. The approach was applied to square windows of 3, 5, 7, 9, 11, 13, 15 and 29 cells, at the finest resolution, each cell is 100-by-100 meters. The last neighborhood (29) was only used to evaluate the sensitivity of this approach. The use of the different neighborhood sizes or map resolutions, allows to gauge the map results sensitivity to scale variation and to find key map resolutions in case of map behavior changes. A two-step process converts the fine-resolution cells to coarse hard-classified cells. For the first step, the size of the coarse cells is determined by aggregating several fine resolution cells. The resolution of the coarse cell is expressed as a multiple of the length of the side of a fine resolution cell. For example, a neighborhood size of 3 means that a 3-by-3 block of fine resolution pixels are aggregated to form one coarse cell. For the second step, a single category is assigned to the coarse cell, based on the majority category among the fine-resolution cells that constitute the coarse cell. For this purpose the application, GridStat software was developed. It results from a refinement of the majority function of "Neighborhood Statistics" in ArcGIS ™ Spatial Analyst. The majority function in "Neighborhood Statistics" is very similar to the mode. Majority computes the value that occurs most often in the neighborhood but has a flaw: when a tie occurs the processing cell is classified as No Data. GridStat Mode will classify the same cell either with its original value or with the closest category. Map algebra and contingency tables were then used to obtain the difference between each of the two maps and create a classification of their differences. For quantification of map comparison approaches, Kstandard and Klocation and binary classification were used (see Fig. 5.3). Khisto was not calculated in this approach since it can be calculated through Kstandard and Klocation.

5.2.4 Soft neighborhood comparison

For computing fuzzy map comparison the module VALIDATE in Idrisi Kilimanjaro® GIS software was used. The module computes statistics for different resolutions (i.e. length of a fine grid cell size) starting from the resolution of the raw data (finest resolution) to a very coarse resolution. An arithmetic sequence was used to create the aggregating neighboring cells into an increasing coarse grid (from 3 to 29 grid cells). We computed until the grid-cell size of 29 to allow comparing with the previous approach.

For maps with one single strata/sub-region VALIDATE computes five especially important numbers for each resolution, that constitute the basis for the components of agreement and disagreement between the reference map and other maps that have increasingly accurate information, from no, to medium and perfect information: i) correct due to change, ii) correct due to quantity, iii) correct due to location, iv) error due to location, and v) error due to quantity. Each cell has partial membership in any of the categories, and the agreement for category *j* in cell *n* is to be the minimum of proportion of category *j* in grid cell *n* of Map 1 and proportion of category *j* in grid cell *n* of Map 2. VALIDATE module also computes the Kstandard and Klocation.

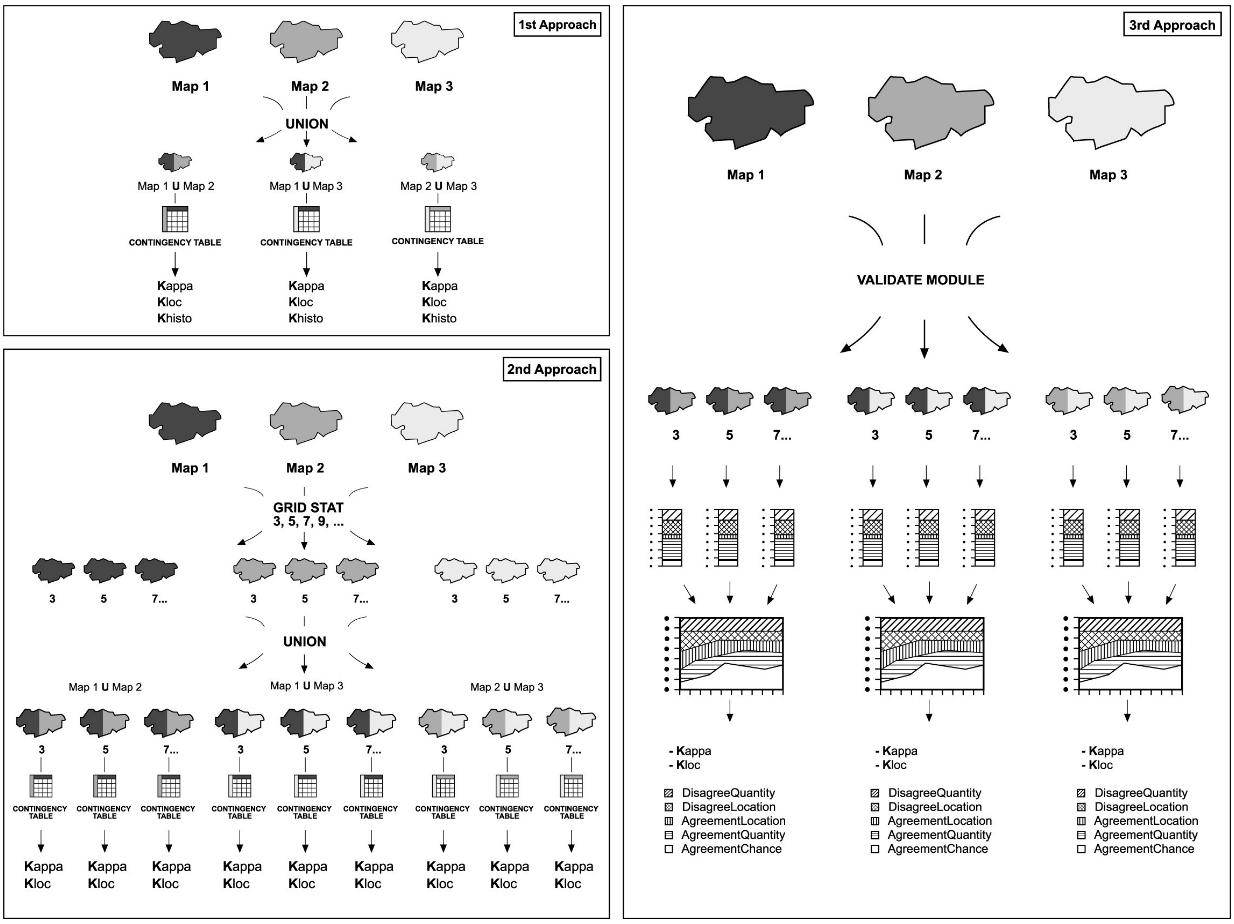

Figure 5.3 – Approaches used for map comparison.

For a more detail and understanding of all VALIDADE calculation, see Pontius (2000), Pontius (2002) and Pontius and Suedmeyer (2004) or for specific application into this study see Caeiro *et al.* (2003c) – Annex Annex V.2).

5.3 RESULTS AND DISCUSSION

5.3.1 Single cell comparison

Analysis of the Kappa values of the three map comparison shows almost perfect agreement between Maps 2 and 3 (Kstandard = 0.85), confirmed not only for quantity (Khisto = 0.89), but also for location similarity (Klocation = 0.95). This result was expected since method 3 is a refinement of method 2. Method 3 is moderately similar to method 1 (kstandard = 0.55). These maps are computed using different multivariate geostatistics but method 3 uses results from method 1. Maps 1 and 2 are the ones with less agreement (kstandard = 0.42) since the computed management units use independent interpolation techniques. Looking at the Klocation value of Maps 1 and 2 (0.51) the differences between these two maps are mainly due to spatial location rather to quantitative dissimilarities (Khisto = 0.83). Binary comparison between Maps 1 and 2 in Fig. 5.4 (above) also confirmed this local difference due to fewer areas of agreement classification. This major location difference can also be true for the Map 1 and 3 comparison since the Klocation value (0.55) is further away from the maximum value than Khisto (0.87). On the other hand, the small difference between Maps 2 and 3 may be due to the quantity category values since the Kloc value is close to maximum similarity (Table 5.1). The refinement of Map 3, i. e. the use of probabilities of the indicator kriguing in the discriminat analysis, seems to compute mainly small differences in quantity, compared to Map 2. Nevertheless all Klocation values show agreement substantially greater than the agreement expected due to chance (Sousa *et al.*, 2002 – Annex V.1).

Table 5.1 – Kstandard and Klocation for the different resolutions and according to hard and soft classification (maximum similarity = 1) (Adapted from Caeiro *et al.*, 2003c – Annex V.2).

Maps comparison			**1 and 2**	**1 and 3**	**2 and 3**	**1 and 2**	**1 and 3**	**2 and 3**
Kappa			**Kstandard**			**Klocation**		
Resolution	1	Hard or Soft	0.42	0.55	0.85	0.51	0.63	0.95
	3	Hard	0.42	0.55	0.85	0.5	0.63	0.95
		Soft	**0.38**	**0.51**	**0.83**	**0.47**	**0.6**	**0.94**
	5	Hard	0.42	0.55	0.83	0.51	0.64	0.95
		Soft	**0.37**	**0.50**	**0.82**	**0.46**	**0.59**	**0.94**
	7	Hard	0.42	0.56	0.83	0.51	0.64	0.95
		Soft	**0.36**	**0.5**	**0.8**	**0.46**	**0.59**	**0.94**
	9	Hard	0.34	0.47	0.77	0.52	0.58	0.95
		Soft	**0.37**	**0.5**	**0.8**	**0.48**	**0.6**	**0.94**
	11	Hard	0.4	0.54	0.81	0.5	0.63	0.95
		Soft	**0.34**	**0.48**	**0.78**	**0.44**	**0.58**	**0.94**
	13	Hard	0.38	0.53	0.8	0.49	0.62	0.95
		Soft	**0.35**	**0.49**	**0.78**	**0.46**	**0.60**	**0.94**
	15	Hard	0.37	0.53	0.78	0.48	0.64	0.95
		Soft	**0.34**	**0.47**	**0.77**	**0.45**	**0.58**	**0.94**
	29	Hard	0.44	0.56	0.78	0.52	0.74	0.98
		Soft	**0.39**	**0.52**	**0.73**	**0.55**	**0.68**	**0.97**

5.3.2 Hard neighborhood cell comparison

The Kappa values (Kstandard and Klocation) do not vary significantly along an increase of neighborhood cells as confirmed by observation of Table 5.1. On average, Kappa values are almost constant up to a neighborhood cell size of 9. This cell size (900 x 900 m) corresponds to less than double the grid sampling size (500 x 750). For cell sizes larger than 9 the Kappa values tend to decrease, i.e. the differences between the maps increase. This is due to a greater number of neighborhood cells and, thus, the inclusion of cells of homogenous areas with a different organic content category (categories from 1 to 4, Fig. 5.2).

Only for neighborhood values that are too high (29 cells, i.e. 2900 m) does the agreement between methods increase more considerably (Fig. 5.4, Table 5.1), since the smaller areas almost disappear. This window size of neighborhood cells (29) is disproportional since it is almost four times larger than the size of the grid sampling cells.

The map comparison taking into account the hard neighborhood cells emphasizes the distinctions between methods, such as areas with more variation within the estuary. These areas are in the opposite direction to water flow (30º), in locations with less hydrodinamics subject to different pollution sources like on the north side of the estuary (Caeiro *et al.*, 2003a – Chapter 4) (see for example the map comparison between methods 1-3 (nb 15) in Fig. 5.4).

5.3.3 Soft neighborhood cell comparison

At the finest resolution (original maps) the overall correct proportion is 58 %, 68 % and 89 %, for comparison between Maps 1 and 2, 1 and 3 and 2 and 3, respectively. A large percent correct is not necessary an important criterion to judge classification schemes because a large portion of percent correct can be attributable to chance (Pontius, 2000). In the case of comparison between Maps 1 and 2, the proportion of disagreement is mainly due to location errors (30 %) and only 12 % is due to quantity disagreement. Also the differences between Maps 1 and 3 are mainly due to location disagreement (23 %) when compared to quantity disagreement (9 %). Comparing Map 1, with Maps 2 and 3, Map 3 is in more agreement, not only as quantity but also as location (Fig. 5.5a), 5.6a), and Table 5.1), for the same reasons explained earlier.

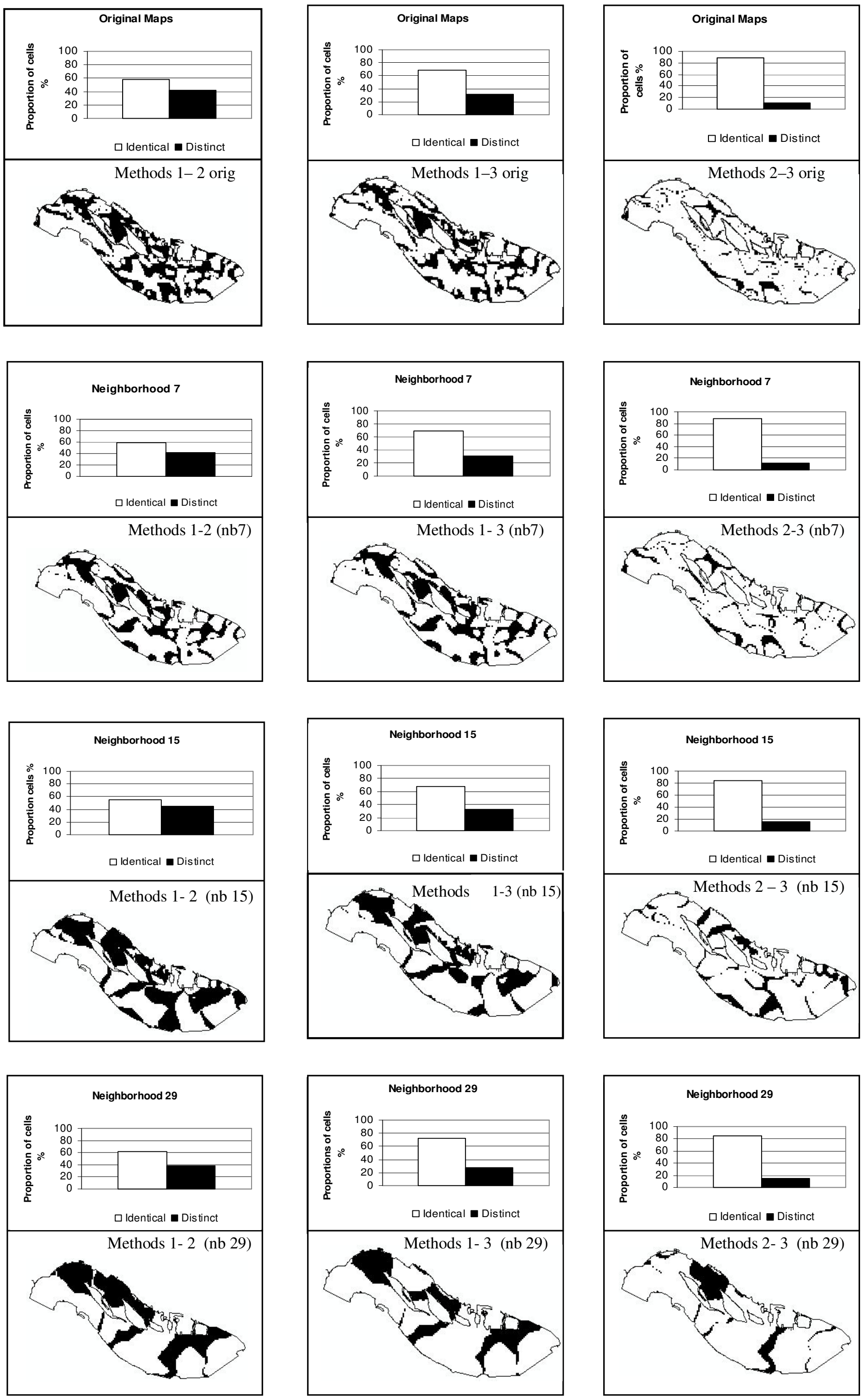

Figure 5.4 – Map comparison for Maps 1, 2 and 3 using Binary classification for single cell and hard neighborhood cells 7, 15 and 29.

In contrast, in the more similar Maps (2 and 3) the small differences are due to quantity (8 %), compared to only 3 % due to location disagreement (see Fig. 5.7a) and Table 5.1). These results are in accordance with Kappa values obtained in the previous approaches.

Figures 5.5b), 5.6b) and 5.7b) show how percent agreement increases as resolution becomes coarser from 1 to 29 grid cells per side of each coarse grid cell, for all method comparison. At the finest resolution, percent correct due to chance is 25, in all the figures, since there are four categories. As resolution becomes coarser, agreement owing to chance tends to increase, agreement due to location decreases, agreement due to quantity doesn't change substantially (or tend to zero in comparison Maps 1 and 2, and 1 and 3), and disagreement due to location decreases. Disagreement due to quantity remains constant since changing the resolution does not change the quantity when the soft (fuzzy) aggregation method is used. Both disagreement and agreement due to location decrease as resolution becomes coarser, because location is less important at coarser resolutions.

a) b)

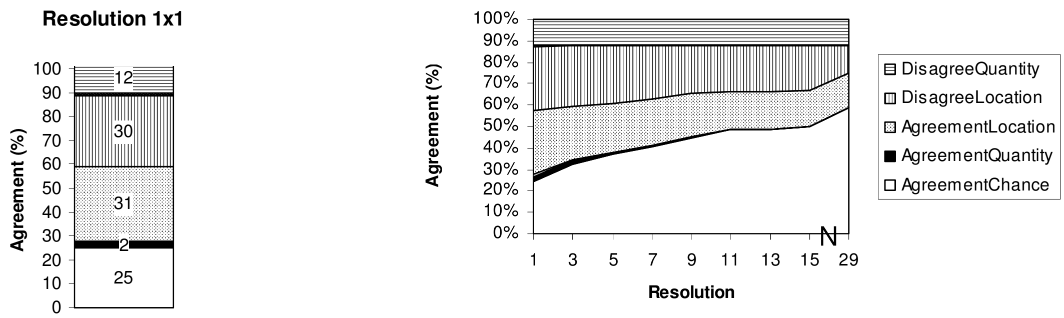

Figure 5.5 – a) Cumulative percent of agreement at fine resolution and b) classification versus resolution for the agreement, between Maps of method 1 and 2 (adapted from Caeiro *et al.*, 2003c – Annex V.2).

a) b)

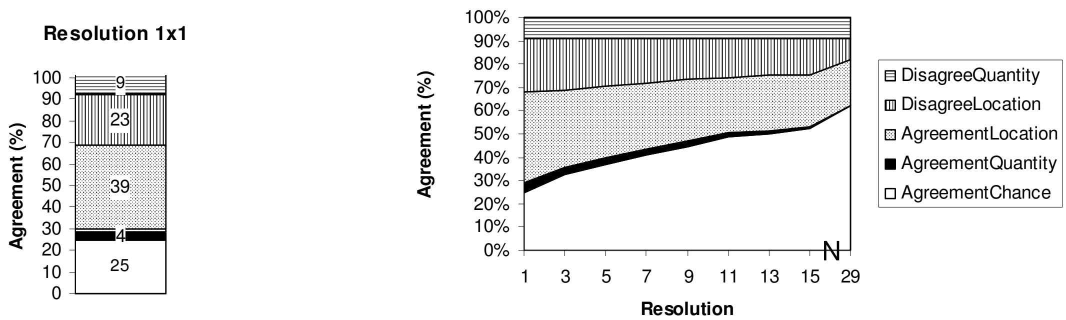

Figure 5.6 – a) Cumulative percent of agreement at fine resolution and b) classification versus resolution for the agreement, between Maps of method 1 and 3 (adapted from Caeiro *et al.*, 2003c - Annex V.2).

The percent agreement between Maps 1 and 2 increases from 58 to 75 % as one moves from the finest resolution to the coarsest resolution. On those maps at finest resolution the Kstandard decreases until the grid cell size reaches 15 and Klocation slightly decreases until grid cell size 7, and increase in the following grid cell (9) and on the coarser one (Figs. 5.5b), 5.8 and Table 5.1).

a) b)

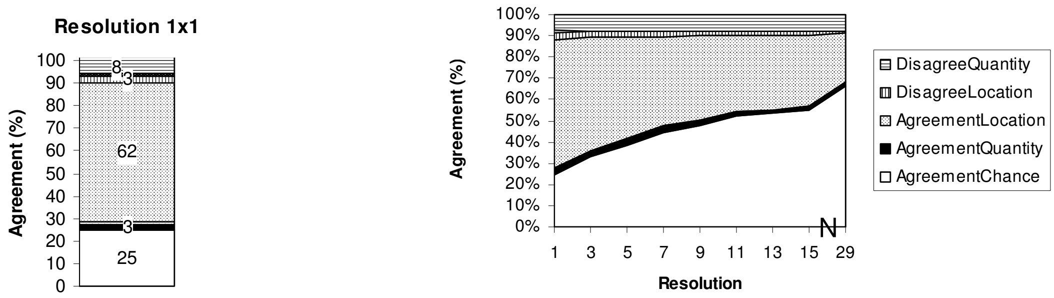

Figure 5.7 – a) Cumulative percent of agreement at fine resolution and b) classification versus resolution for the agreement, between Maps of method 2 and 3 (adapted from Caeiro *et al.*, 2003c - Annex V.2).

As resolution becomes coarser, percent agreement between Maps 1 and 3 increases from 68 to 81.7 %. As resolution becomes coarser Kstandard slightly decreases until grid cell size 15 and Klocation slightly decreases until grid cell size 7, and increases in the coarser grid cells having is higher value (0.68) (Figs. 5.6b), 5.8 and Table 5.1).

a) b)

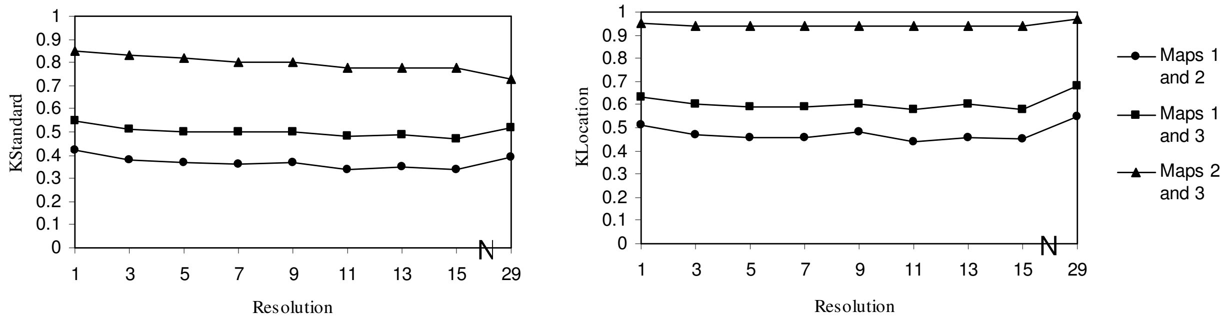

Figure 5.8 – a) Kstandard and b) Klocation for the different resolutions, calculated using fuzzy classification (adapted from Caeiro *et al.*, 2003c – Annex V.2).

For both comparisons of Maps 1 and 2 and Maps 1 and 3 the disagreement due to location at resolution 7 is about 90 % of the disagreement due to location at resolution 1, indicating that only 10 % of the disagreement due to location happens over distances less than 700 m. This grid cell size is similar to the sediment sampling's grid used for computing the maps (750 x 500). This sampling grid was calculated with the principle that there are not important differences in sediment characteristic at distances smaller than the sampling grid (Caeiro, *et al.,* 2003b – Chapter 3).

The percent of agreement between Maps 2 and 3 increases from 89 to 91.6 %, as one moves from the finest resolution to the coarsest resolution. The Kstandard decreases as resolution becomes coarser and Klocation is almost constant, only slightly increasing at the coarser resolution (Fig. 5.8b).

As well as in hard comparison only for the coarser resolution (29 cells, i.e. 2900 m) does the agreement between methods increase more significantly (see Fig. 5.8 and Table 5.1), with the exception of Kstandard of map comparison between Map 2 and 3.

Comparing hard with soft comparison it is noticed that for comparison between Map 1 and 2 and Map 1 and 3 values of Kstandard calculated through hard comparison classification show higher variation than the ones calculated through soft classification. This is specially noticed at cell size 9 (see Table 5.1) as already stressed in 5.3.2 Chapter. The influence of the hardening step is likely to be the source of this more pronounced variation. Similarly, values of Klocation obtained with hard comparison classification are slightly higher then the ones computed through soft classification. The maps look more similar in terms of location using the hard classification compared to the fuzzy classification since hard classification reclassify each grid cell at map resolution according to Mode function.

5.4 CONCLUSIONS

In this paper we used different map comparison approaches to compare spatial models of estuarine sediment management units. All of the approaches although with disadvantages can complement each other.

Since the sixties the map comparison technique was assessed using Kappa index of agreement. However Kstandard fails to penalize to not give intermediate similarities and to attribute correct classification to chance. Also fails to penalize for large quantification error and fails to reward sufficiently for small quantification error. In addition it is unsuccessful to distinguish clearly between quantification error and location error (Pontius, 2000). Nevertheless in this work Kappa gave good, fast and easy information that can be added with other methods, in particular with the new Kappa variants to quantify quantity and location errors. Also the binary classification gave a fast and easy visualization comparison.

The classification schemes that attempt to specify accurately both quantity and location are better to evaluate the marginal distributions in a spatial model. Here we presented a new methods (3rd approach) of accuracy assessment to budget the component of agreement and disagreement in terms of quantity and location between any two maps that show a categorical variable. This assessment can be done not only at raw map resolution but also at multiple resolutions using fuzzy classification (Pontius and Suedmeyer, 2004). By using the minimum proportion of each category, in each grid cell, the results are the proportion of a category that is within the same pixel as another category. This allows fuzzy agreement maps containing more information and giving an easier and realistic interpretation of the dataset, when compared with hard comparison. Despite this the results although easily computed in the software and represented in a simple graphical form, can be tricky to interpret. Also similar conclusions were obtained about the maps differences using either Kappa indices or the component of agreement.

The hard classification can cause changes in the quantity of each category, leading to misleading results. Even so, hard neighborhood comparison may be useful for an easy visualization of map overlays (like Fig. 5.4) as a criterion for defining a reduced number of these management units for a future extended management program of this estuary. Coastal Zone management represents a dynamic process which develops and implements a co-ordinated strategy to allocate resources to achieve the conservation and sustainable multiple use of coastal zones (French, 1997). A reduced number of management units provides a model of estuary management that is more appropriate, easier to manage and less expensive to monitor.

The different comparison approaches demonstrated that using either single cell, neighborhood hard or soft comparison, although giving different interpretation, the three estuarine management unit's maps are still similar. The differences are mainly due to location disagreement in case of comparison of Map 1 with Maps 2 and 3. This helped to conclude that the use of different geostatistical multivariate methods mainly computed differences in spatial patterns. Also these different comparison approaches helped to consolidate the lack of benefit of using the indicator kriging probabilities of the method 1 into method 2, resulting in method 3 as stated in Caeiro *et al.* (2003a) – see Chapter 4. Finally it also confirmed the choice of Method 1 that seems to better represent the spatial pattern of the four categories of organic load.

All the results reinforce the robustness of management unit's calculation. Moreover the results, support the choice of any of the methods as equivalent and thus of equal value for environmental management. Hence the likelihood of map resulting from method 1 being a bad choice is weakened.

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PART IV

SOCIAL AND ECONOMICAL PRESSURES

CHAPTER 6 – APPLICATION OF THE DPSIR MODEL TO THE SADO ESTUARY IN A GIS CONTEXT – SOCIAL AND ECONOMICAL PRESSURES

APPLICATION OF THE DPSIR MODEL TO THE SADO ESTUARY IN A GIS CONTEXT – SOCIAL AND ECONOMICAL PRESSURES

Caeiro, S., Mourão, I., Costa, M. H., Painho, M., Ramos, T. B., Sousa, S. (2004)

F. Toppen, P.Prastacos (Ed.) *Proceedings of 7th AGILE Conference on Geographic Information Science* 29 April - 1 May, Greece, Heraklion, pp. 391 – 402.

ABSTRACT

Finding the most appropriate tools that help to assess and manage the estuarine environments, allowing their restoration, are one of the main issues in coastal zone management. This paper describes the application of the DPSIR (*Driving Forces-Pressures-State-Impact-Response*) indicators framework to an estuary in Portugal based on a Geographical Information System (GIS). The work is focused on a preliminary identification and evaluation of the social and economical pressures. Within the Sado Estuary, Setúbal sub-watershed was chosen as case study. The indicators are further calculated and discussed for an overall assessment.

KEYWORDS: Sado estuary, DPSIR Model, Indicators, GIS, Social and economic pressures.

6.1 INTRODUCTION

The coast is a difficult place to manage, involving a dynamic natural system which has been increasingly settled and pressurised by expanding socio-economic systems (Turner, 2000). A study that integrates the socio-economic variables establishes which problems and opportunities are present in a coastal area, why coastal zone management is needed and what its goals and objectives should be (Cicin-Sain and Knecht, 1998).

The DPSIR Model, adopted by the European Environmental Agency, is one of the frameworks based on the concept of causality chains for data synthesis, which links environmental information using indicators of different categories (*Driving forces, Pressure, State, Impacts and Responses*) (UNEP/RIVM, 1994, RIVM, 1995)(Fig. 6.1). This model is similar to the PSR (*Pressure-State-Response*) framework (OECD, 1993), but with two more categories: *Driving forces* and *Impacts*. The first reports to the “needs” of individuals and institutions that lead to activities that exert pressures on the environment. *Driving forces* are understood as the social needs that require the existence of a given economic activity. The "intensity" of the *Pressure* depends on the nature and extent of the *Driving forces* and also on other factors which shape human interaction with ecological systems. The *Impacts* are related to ecosystems and human health due to *State* modifications. The policy *Responses* lead to changes in the DPSIR chain. Greeuw *et al.* (2001), stated that one problem of this framework is that the same item can appear in different places, depending upon which target we are focusing on. Also according to Kelly (1998), the framework fails to capture the complexity of the relationships in complex systems. Nevertheless it is a model largely used and if these drawbacks are taken into account, it could work as a good tool to support the management of ecosystems. Also, indicators are an excellent way of representing the environmental components avoiding the measurement of too many parameters. Indicators are often adopted to avoid and reduce the complexity of environmental data. In general, indicators are easily quantified and delineated from already described information in protective goods like environmental compartments and are adequate to assess what is called ecosystem health (Costanza, 1992).

The DPSIR framework can be used as a base for coastal zone environmental management allowing the linkage between environmental and macro-economic models, making it possible to integrate the conservation functions (biodiversity and ecological) with socio-economic development (RIVM, 1995). The application of this causality models in a GIS context has the advantage of allowing the spatial visualization and better integration of the different indicators. Zandbergen (1998) used an integrated approach to link key pressure indicators and GIS maps to visualize complex information what was well received as a decision support tool. The use of these models of causality chains and the selection of the indicators has often been applied in coastal zone management in the last decade. Examples could be: Cooley *et al.* (1996), Ward *et al.* (1998), Chesapeake Bay Program/USEPA (1999), EEA (1999), ME (2001), Casazza *et al.* (2002), Elliott (2002), Jorge *et al.* (2002), Silva and Rodrigues, (2002), Nunneri and Hoffman (2003), Picollo *et al.* (2003), among others. However some of these approaches are only conceptual or little attention is paid to the difficulties of calculating the indicators and their spatial visualization and interpretation for future management of the coastal zones. This fact is of particular importance in the case of social and economic pressures indicators.

This paper illustrates the practical application of the DPSIR model to the Sado Estuary. This estuary, located in the west coast of Portugal is an area where management conflicts are known: although it has a high ecological value, fact that is highlighted by the existence of a Natural Reserve (RNES), it is a very industrialized and populated zone. Therefore, it becomes necessary to build and implement environmental assessment models, which include the construction of methodologies and frameworks that, qualitatively and quantitatively, define the state of coastal area and point out management options.

The main aim of the research project, in which this work is included, is the development of a framework for an estuary environmental data management using the DPSIR Model, including collection, processing and analysis of data, through a GIS. This paper describes the preliminary results of the quantitative analysis of the two first model categories *Driving forces* and *Pressures* indicators. One of the Sado's river sub-watersheds was used as example.

6.2 METHODOLOGY

6.2.1 Previous work

The methodological approach of this research project is briefly described in Fig. 6.1. Collection of information about the different conceptual frameworks for indicators (Ramos *et al.,* 2004) and compilation of all kind of data related with the Sado Estuary were the initial tasks. DPSIR model was them elected as the assessment tool and a preliminary set of indicators for each of its components was selected (Caeiro *et al.*, 2002 – Chapter 2).

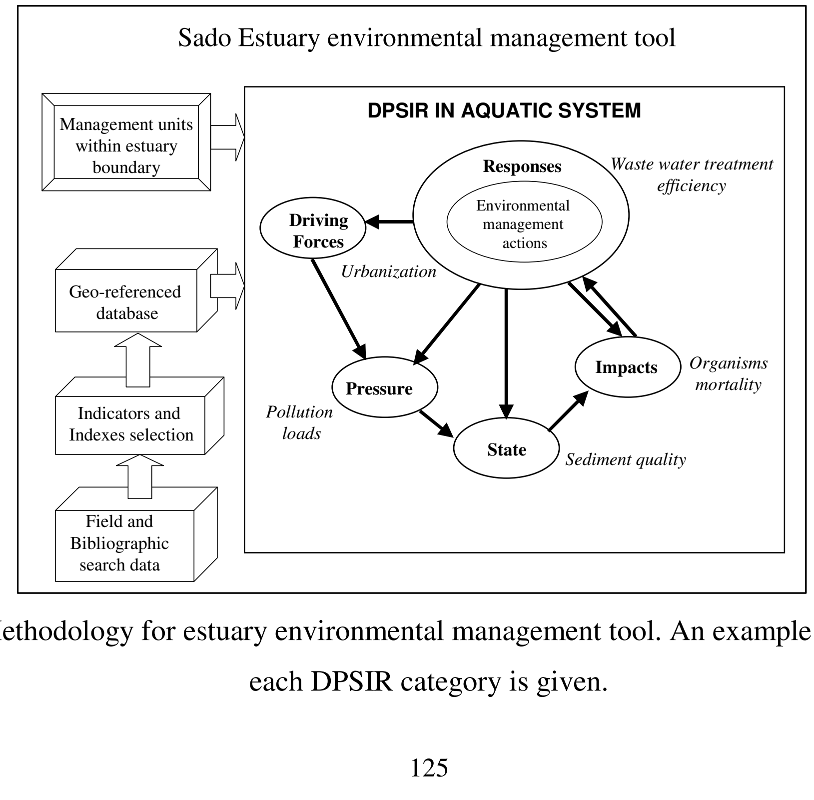

Figure 6.1 – Methodology for estuary environmental management tool. An example of an indicator for each DPSIR category is given.

The methodology proposed for the environmental management system applied to the Sado Estuary supported on the DPSIR framework, is based on identifying, representing and characterizing a series of homogeneous environmental areas inside the estuary (Caeiro *et al.,* 2003a – Chapter 4). On each of these management units, *State* and *Impact* indicators are going to be quantified. These areas are then to be linked with the social and economic pressures measured in the estuary itself and in the terrestrial boundaries of the surrounding areas (*Driving forces* and *Pressures* indicators).

This management system will allow the integration between the biodiversity conservation and human pressure for development. The methodological approach to integrate this information will be the implementation of a GIS.

6.2.2 Driving forces and Pressures evaluation

After the selection of the *Driving forces* and *Pressure* indicators the data was collected in different institutions in Portugal, or searched in literature, for their quantification. The set of selected indicators that were chosen for the *Driving forces* and *Pressure* categories and source of information are listed in Table 6.1. An indicator's preliminary calculation and spatial representation was conducted. However, some indicators are not yet calculated or georeferenced due to the current unavailability of the data. The evaluated indicators are highlighted in Table 6.1 (lines with shading).

In terms of pollution loads, only the locations of the urban Wastewater Treatment Plants (WWTP), their type of treatment (primary, secondary or tertiary), the location of the wastewater discharges and a qualitative evaluation of the contaminants discharged were available. For the urban wastewater discharges and non-point sources it was possible to quantify the pollution loads in terms of Biological Oxygen Demand (BOD), Nitrogen (N), Phosphorous (P) and Total Suspended Solids (SS) loads. In the case of urban point sources the loads were estimated based on bibliographical information concerning emission factors per capita (Tchobanoglous, 1995).

The GIS was developed in *ArcMap 8.1*. It was simultaneously a means to visualize data and a calculation tool for indicators that were related to geographical information. Watershed areas were chosen as the terrestrial units for indicator representation. Setúbal sub-watershed was elected as an example for the calculation of the indicators since the main human pressures of the estuary are located in this area (Fig. 6.2). The indicators were overlaid within the coastal area shoreline (Caeiro *et al.,* 2003b – Chapter 3).

Table 6.1 – Selected indicators, unit, GIS representation and source of information. Evaluated indicators are in italic.

Driving Force Indicators	Unit	GIS Representation	Source of Information
Urban areas near the estuary	*km^2*	*Area*	*Portuguese Geographical Institute: IGEO (2003)*
Industry types[1]	*number of establishments per industry type*	*Point*	*Technical/scientific data Correia and Florêncio (2002)*
Dunghills/ sanitary landfills	km^2	Area	National Waste Institute (INR)
Rice-fields	*km^2*	*Area*	*IGEO (2003)*
Salt-pans[2]	*km^2*	*Area*	*RNES, Technical/scientific data: Painho et al. (1996) and Dias (1994)*
Aquacultures[2]	*km^2*	*Area*	*RNES, Technical/scientific data: Painho et al. (1996) and Dias (1994)*
Fishing[3]	*number of fishing ships per harbour. year^{-1}*	*Point*	*Ministry of Agriculture and Fishery (MAP)*
Ships traffic	*number of ships per harbour. year^{-1}*	*Point*	*Setúbal and Sesimbra Administrative Port APSS (2003a)*
Harbours	*number*	*Point*	*APSS (2003a), IGEO (2003)*
Tourism areas	km^2	Area	Statistics National Institute (INE)
Pressure Indicators	**Unit**	**GIS Representation**	**Source of Information**
Population density	*inhab.km^{-2}*	*Area*	*INE, 2003*
Toxic substances spill	number of spills occurrence. year^{-1}	Point	Maritime Police
Pesticides in rice-fields	t.ha^{-1}.year^{-1}	Area	Technical / scientific papers
Fertilizers in rice-fields	t.ha^{-1}.year^{-1}	Area	Technical / scientific papers
Commercial species captured (fish and bait)[4]	*t fresh weight.year^{-1}*	-	*MAP*
Dredging[5]	*m^3.year^{-1}*	*Point*	*APSS (2003b)*
Dredged material disposal[5]	*m^3.year^{-1}*	*Point*	*APSS (2003b)*
Urban wastewater discharges without suitable treatment	*m^3.year^{-1} or t contaminant. year^{-1}*	*Point*	*Water Institute: INAG, (2001) Technical/scientific data: Correia and Florêncio (2002).*
Industrial wastewater discharges without suitable treatment	*m^3.year^{-1}or t contaminant. year^{-1}*	*Point*	*Technical/scientific data: Correia and Florêncio (2002) AQUA/FCT/UNL (1997)*
Solid waste disposal	t.year^{-1}	Area	INR
Solid industrial waste disposal	t.year^{-1}	Area	INR
Non source pollution (water runoff)[5]	*t.year^{-1}*	-	*Technical/scientific data: INAG (2001)*

[1]Only number of industries was represented; [2]Not available geographically which are salt-pans or aquaculture. Data of Setubal and Alcacer do Sal Municipalities; [3]All the existent fishing dock were considered and not only the ones at Setúbal sub-watershed area [4]Only the fish data is available; [5]Spatial data is not available.

A Standard approach, i.e. normalization factors, were used to express the results of the environmental indicators like for example total sub-watershed area, total estuary area or coastline length were used as denominators. This normalization allows comparison between indicators and with other costal zones. It also allows a better evaluation of the level of their magnitude. The estuary area (water area) considered in this study was the area of the main bay until the entrances of the Águas de Moura and Alcácer Channels (about 56 km^2). When available, a temporal evolution of the indicators was also performed.

The different indicators of *Driving forces* and *Pressures* categories were visualised and evaluated together for a better integrated assessment of the human activities and related pressures in the estuary. Not all the *Driving forces* indicators have one-to-one linkages with the *Pressures* indicators. An integrated approach should be adopted relating different indicators as clusters with multiple aspects that interact with each other (Ramos *et al.,* 2004).

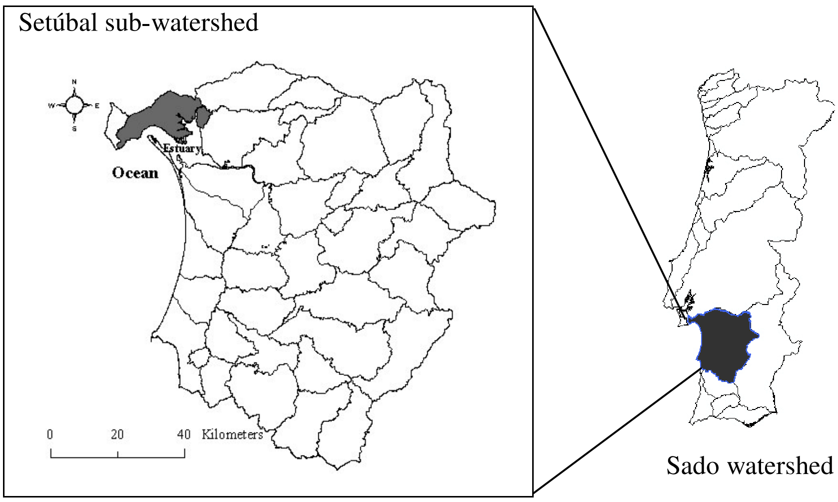

Figure 6.2 – Sado watershed. Adapted from INAG (2001).

6.3 Results and discussion

The main Setúbal sub-watershed urban, agriculture and industrialized pressures in the estuary are shown in Fig. 6.3. The qualitative evaluation of the effluent discharges is shown in Fig. 6.4. Evidence shows that high pressures exist in the North Channel of the estuary.

The urban use has an area of approximately 10.3 km^2, corresponding to 4.5 % of the sub-watershed total area, distributed by 11 villages. This sub-watershed has many urban areas because the main city (Setúbal) is located in it. As can be noticed from Fig. 6.3 the population density is higher near the estuary boundary (see Table VI.1 – Annex VI).

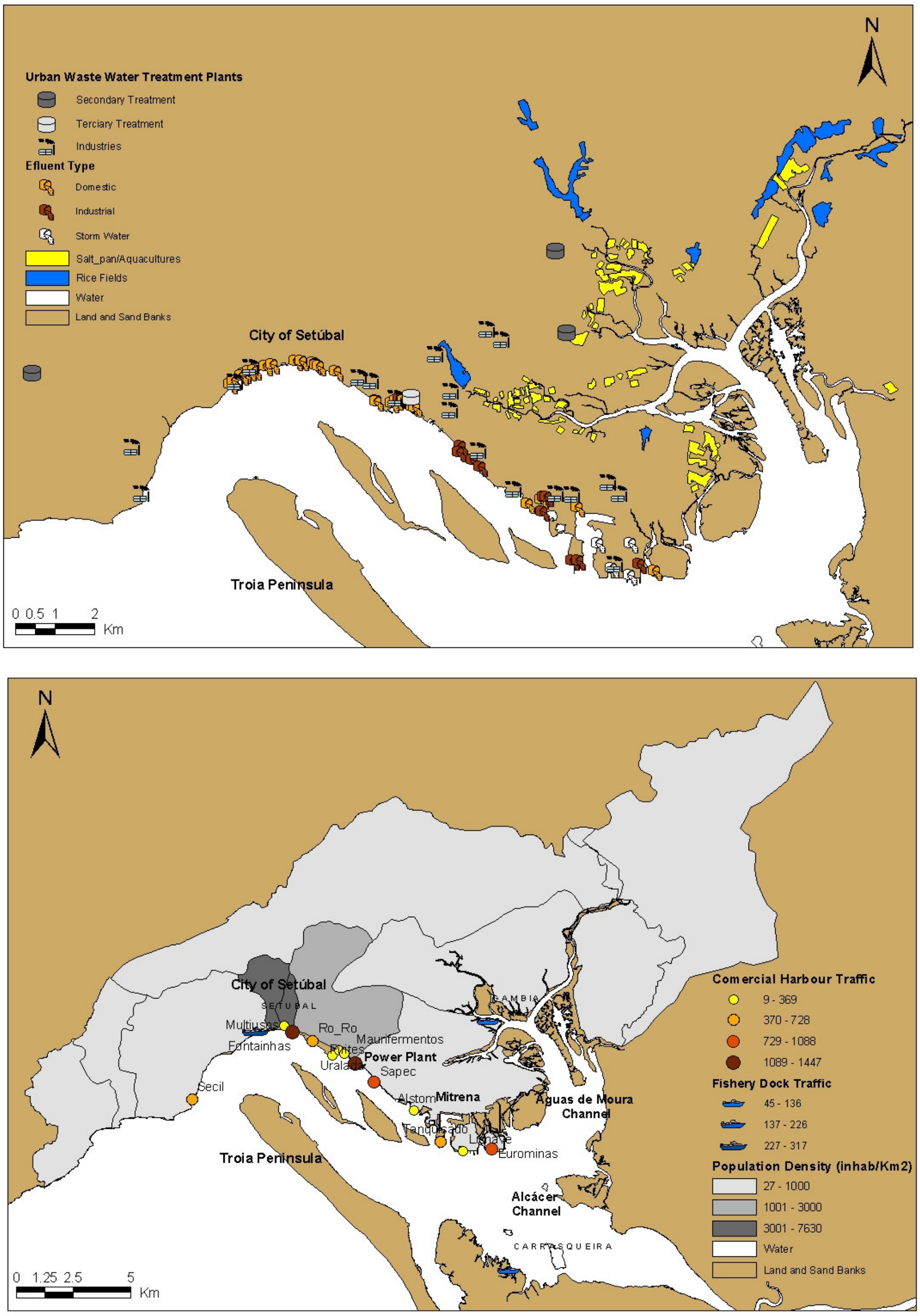

Figure 6.3 – Urban, agriculture and industrial indicators in the Setúbal sub-watershed. In industrial effluents are included industrial, storm water and/or domestic wastewater. In domestic effluents are included domestic and/or storm water. Average traffic of ships (nº ships/year), from 1999 to 2003, in the main commercial harbours and average traffic of fishing ships, from 1998 to 2002, in the fishing docks Population density of 2002 year.

A large and dense number of urban and industrial effluents are discharged into the estuary. In the zone of higher population density (Setúbal City) the major wastewater discharges are urban. The presence of industries is followed by industrial wastewater that discharge their effluent into the estuary. Near Lisnave shipyard, Tanquisado and Eurominas industries there are also storm water effluents. On some of these effluents it is possible that runoff results not only from rainfall but also from contaminated water associated with the industrial activities. It was not possible to assess, with the necessary accuracy, i) if each industrial effluent discharge has suitable treatment, ii) where each urban WWTP discharges their effluents, iii) what are their capacities and iv) what are the treated wastewater characteristics. Only the WWTP near Setúbal has tertiary treatment, and started to operate only recently. Some of the industries will also be connected to this plant (like SAPEC - fertilizers and pesticides and Maurifermentos - ferments) which, at the moment, don't have a suitable wastewater treatment. Lisnave shipyard and the power plant industry have their one WWTP but it was not possible to know their efficiency. Industrial complex of Mitrena – (olive oil packaging, plastic manufacturing, cereal storage and reused paper industries) has a WWTP but there is evidence that it is not working properly (APSS – personal communication) (Fig. 6.3).

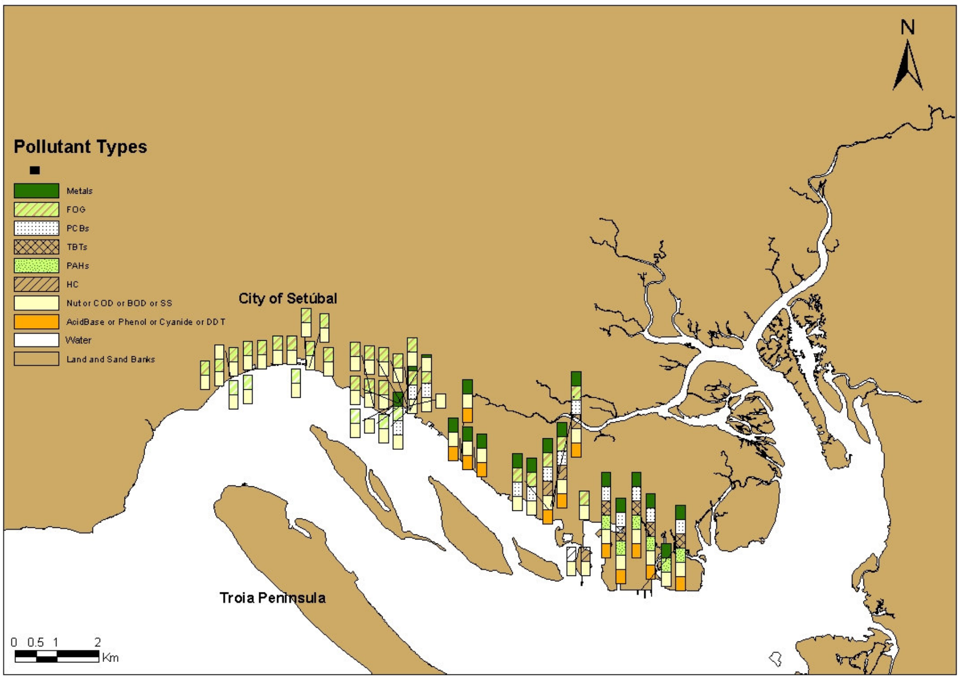

Figure 6.4 – Main pollutant types in each effluent discharge into the Sado Estuary.

The main contaminants agents discharged in the urban effluents are Fats, Oils and Grease (FOG), Nutrients (Nut.), Chemical Oxigen Demand (COD), Biological Oxigen Demand (BOD) or SS. The effluents discharged near Eurominas and Lisnave have more complex mixture contaminants like metals, Polychlorinated Biphenyls (PCB), Tributyl-tin (TBT) and

Polyaromatic Hydrocarbon (PAH) (Fig. 6.4). Most of this contaminants are persistent and toxic to the marine biota (Laws, 1993). Since along the North Channel the hydrodynamics is low, and the more complex contaminants are discharged in Shipyard and Eurominas area, it is expected higher impact in that estuarine area.

The major sources of nutrients (N e P) in the estuary are non-point sources, mostly due to agricultural activities (Fig. 6.5 and Table VI.2 in Annex VI). Nitrogen load is high when compared with Phosphorus and is expected to be higher than P in urban runoff, raw wastewater and rainfall (Laws, 1993). Analyzing BOD and SS, the major input is due to point sources (non-point BOD and SS are only 15 % and 32 % of total sources). Nevertheless special care must be taken when comparing these two pollution sources, since they were calculated based on different methods and sources. It was not possible to represent spatially this data but non-point sources are expected to come mainly from Águas de Moura Channel.

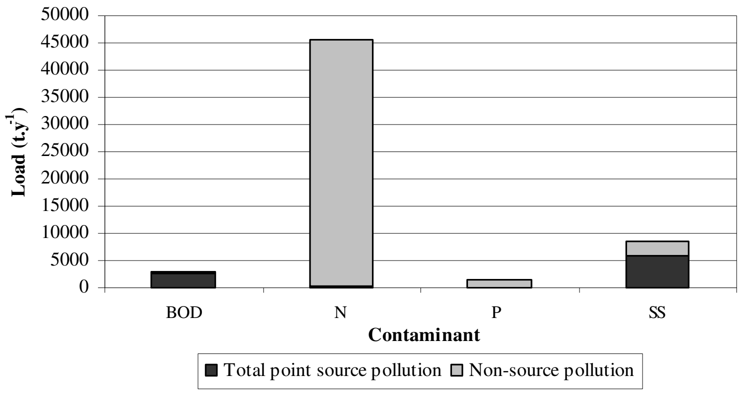

Figure 6.5 – Loads of BOD, N, P and SS from point and non-point sources in the Setúbal sub-watershed.

Salt exploitations area is usually organized by groups of salt-pans (Dias, 1994) (Fig. 6.3). The sum of the area of this *Driving Force* is 8.36 km^2 corresponding to a total of 19 groups distributed along Setubal and Alcacer do Sal municipalities (Table VI.3 in Annex VI). This indicator should also be seen as a positive *Pressure* once the maintenance of salt-pans is a sign of nature conservation and biodiversity. Aquacultures are frequently implemented in old salt-pans (Dias, 1994). This fact can cause difficulties in the spatial representation of this indicator (negative pressure), which needs to be distinguished from the previous indicator (positive pressure). Some old groups of salt-pan areas disappeared to give place to aquacultures, in some cases with larger areas (Fig. 6.6 and Table VI.3 in Annex VI). This replacements and new installations are one of the great concerns of the Natural Reserve since some of these aquacultures use unauthorized intensive culture systems that can cause extra organic loads into the estuary. Furthermore the use of anti-fouling, pesticides, fertilizers, pharmaceutical products and introduction of new species are also aquaculture activities that can cause other important negative impacts (Amaral, 2000).

The rice-fields area in the Setúbal sub-watershed is 4.18 km^2, corresponding to only 1.8 % of the sub-watershed area (Fig. 6.3). The major rice-fields are located on the right side of the sub-watershed upstream Águas de Moura Channel near the salt-pans. This *Driving force* is responsible for important loads of pesticides and fertilizers into the estuary coming from this channel. According to Pereira (2003), pesticides like Endolsulfan, Lindane, Molinate, Propanil, MCPA and Clorphenvinphos are used by rice-field farmers in Sado watershed. In particular, Endolsulfan, Chlorphenvinphos and Molinate have high potential to cause adverse toxic effects to the biota community in Sado river. Also two of the WWTP that are located near Águas de Moura Channel are discharging their effluents into this channel (Fig. 6.3).

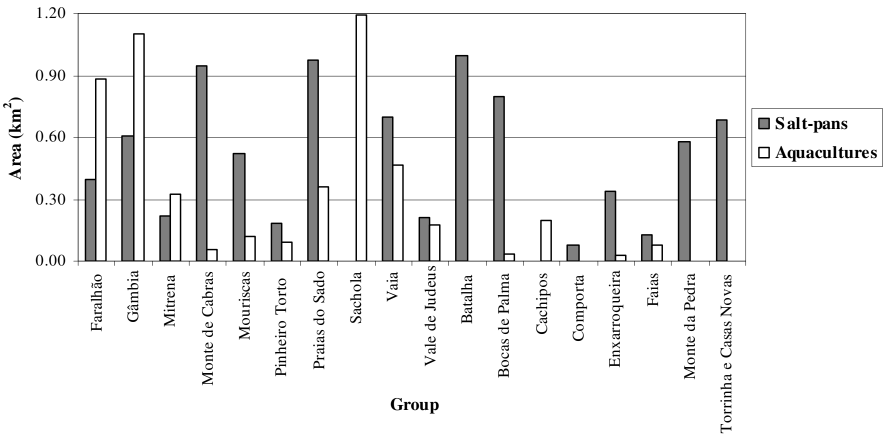

Figure 6.6 – Groups of Salt-pans/aquacultures and their areas in the Sado Estuary.

The Port of Setúbal represents about 10 % of the National port and maritime sector activity (APSS 2003a). The major harbours in the estuary are located on Setúbal's sub-watershed. Inside the study area there are about 20 harbours, most of them industrial. The area occupied by these structures has approximately 0.90 km^2, which represents approximately half of the coastal line occupied by the sub- -watershed, and about 2 harbours per km of coastline. The traffic of ships per commercial harbour, during the period 1999-2003 (average values), is shown in Figs. 6.3 and 6.7. During theses years not an important increase was observed in the traffic of ships in the Sado Estuary (about 115 ships per km^2 of estuary area per year). Pirites and Fontaínhas, followed by Eurominas and Sapec, are the harbours with higher traffic, so the most intense impact in the estuary, due to this *Pressure*, is expected in those locations. Pirites is an industrial harbour where the main cargo types are Cooper concentrates and fuel-oil; Fontaínhas is a marina and recreation boating and Eurominas is an industrial harbour where the main cargo type is coal and clinker (APSS, 2003a). Eurominas industry, although desactivated, is mainly used now for harbour activities, may explain the decrease in ship traffic in the last years. Sapec is also an industrial harbour where the main cargo is petroleum coke, coal, clinker and cereals. Several pollutant loads can be associated with these human activities like BOD, COD, SS, petroleum hydrocarbons, solvents, metals and FOGs (USEPA, 2001).

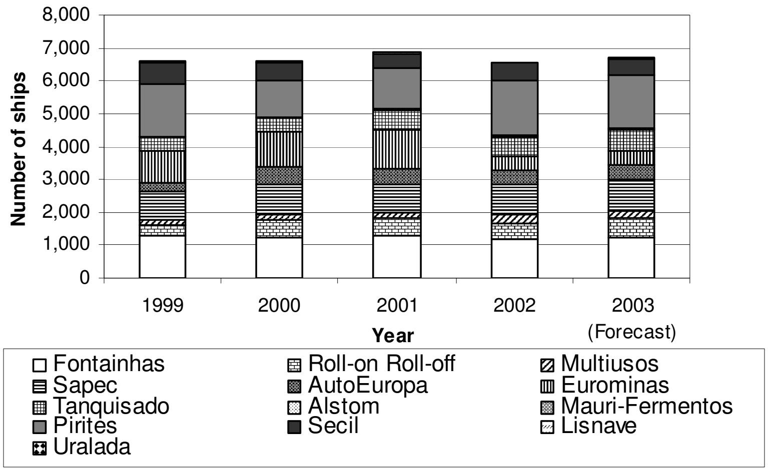

Figure 6.7 – Traffic of ships in the main harbours from 1999 to 2003. Eurominas and Auto-Europa correspond to data for more than one harbour that for simplification reasons was joined.

The fishing dock with higher traffic is Setúbal, compared to the other two (Gâmbia and Carrasqueira) (Fig. 6.3). There was a decrease in the number of boats between 1998 and 2002 years in Setúbal dock, but an increase in the other docks in the year 2002, although not significant in an overall analysis of this indicator (Fig. 6.8 and Table VI.4 in Annex VI). In this last year the fishing boats represented only 6 % of the total traffic of ships in the estuary. As can be concluded from Fig. 6.8, the number of boats and the fish caught yield distinct patterns (Table VI.4 and VI.5 in Annex VI). Since 1998 the number of boats has been decreasing and until 2000 the fish catches increased. This could be related with better catching techniques, higher number of working hours, larger capacity of the fishing boats or others. From 2000 to 2002 both number of boats and fish caught decreased. These latter facts could be related with European Union fishing policies. Nevertheless there is no other information available like number of working hours, fishing fleet characteristics, fish stocks and more complete temporal series that could help a better interpretation of this data.

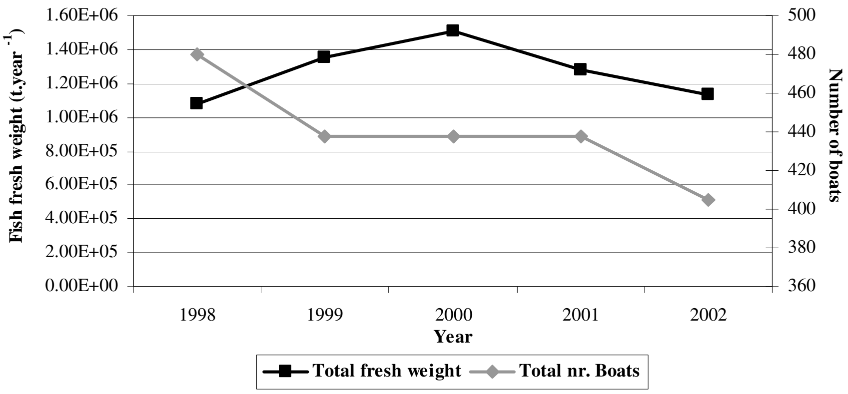

Figure 6.8 – More important commercial fish fresh-weight caught and number of fishing boats from 1998-2003 (average of the 3 docks).

To evaluate the *pressure* indicator fish species caught with commercial value, the data of the three fishing docks were also analysed together since the fish discharged in each dock is not related with the proximity of the catchments area to the dock but with the sale market of each harbour. A slight decrease in some species has been noticed in the weight of each captured species along the analysed period (from 1998 to 2003) (Fig. 6.9). Ray, two-banded sea bream, black bream and grey mullet are the most relevant species captured in the estuary, in terms of fresh weight. These species are abundant in the Portuguese coast, in particular sea bream, which uses the estuary for nursery (Sobral and Gomes, 1997). Among the marine species discharged, sardine and horse-mackerel assume the major relevance, even when compared with estuarine species. Both these marine fishes have high commercial interest due to traditional Portuguese gastronomy. Several studies showed that some of the species with commercial value have been affected by the human activities in the estuary (Antunes and Cunha, 1995, Cunha, 1995). Small shed is a vulnerable species according to "Vertebrate red book of Portugal" and eel is considered a commercially threatened species. Prove of this is their low levels of capture (Fig. 6.9). Toadfish is a resident species of Sado estuary being highly vulnerable to changes in its habitat. Setúbal's inhabitants highly appreciate this fish in their food diets (Sobral and Gomes, 1997). For a better evaluation of the fish resources *Pressure* and their *State* on the estuary, the fish catches should be related with the fish stock. There is still the need for research in this field, since stock data is available for a very few species and only at a national level.

According to APSS (2003b), in the year 2004 maintenance dredging operations will be carried out with an average total volume of 919,186 m^3 dredged material. These dredging operations will be made in the North Channel (from Fontaínhas to Alston harbours – 435.3

m^3), entrance of the estuary (connection between sea and estuary – 404.9 m^3) and South Channel (From Eurominas to Tanquisado – 79.0 m^3). These dredging operations are related with maintenance of the navigation channels and will correspond to about 15 m per km^2 of estuary area. This dredged material will be disposed in Setúbal Canyon, an area outside the estuary with high hydrodynamics. Therefore, it is assumed that this activity will not exert pressure on the study system.

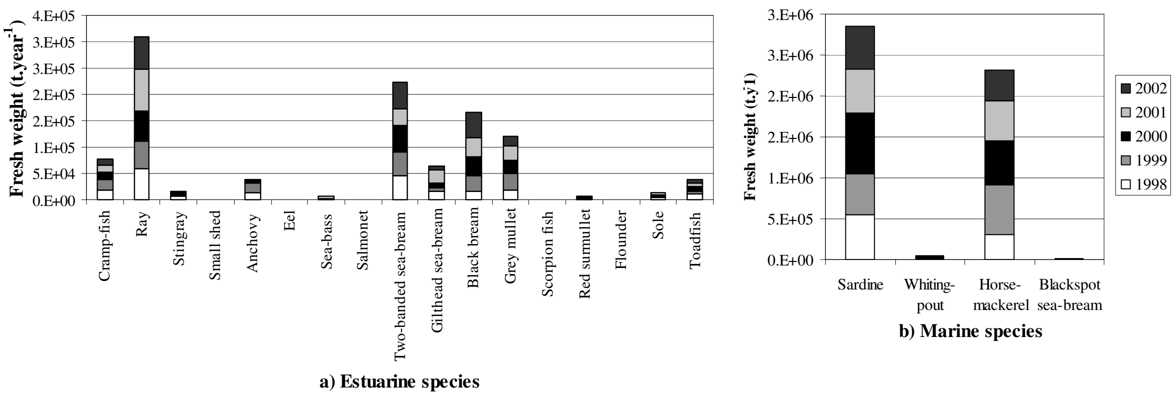

Figure 6.9 – Most important commercial fish species a) estuarine and b) marine) captured in the Sado Estuary and their fresh weight discharged in the period from 1998 to 2002. These values correspond to the average value of the species discharged in the three fishing docks.

6.4 CONCLUSION

In this paper indicators belonging to the DPSIR *Driving forces* and *Pressures* categories were assessed using a GIS. GIS is a useful tool for this kind of data synthesis models since it facilitates the visualization and computation of indicator results. Although only some preliminary results of the indicators were calculated and visualized with the GIS, it already allowed discussing the indicators' information and limitations. Zandbergen (1998) stressed that spatial trends in selected indicators can be illustrated effectively using GIS, which helps to identify particular regions within the watershed which should receive a higher priority for management. This preliminary quantification was a difficult task due to data unavailability. Much of the data, like the pollution loads evaluation, were only possible in a qualitative way. Although several plans and inventories were developed or are in development, most of them performed due to EU obligations, their data is not easily accessible, even for academic purposes.

The *Driving forces* and *Pressures* indicators assessment in the Setúbal sub-watershed lead to the following conclusions: i) existence of clustered populated areas near the city of Setúbal and estuary boundary; ii) existence of a dense number of ports most of them industrial in the North Channel, in which the main cargo movements are a potential source of pollution, like petroleum derivates; iii) existence of industrial, urban and storm water effluents, most of them discharging wastewater without suitable treatment with a diverse type of contaminants; iv) agriculture and aquaculture activities, sources of non-point pollution loads coming from Águas the Moura Channel. Due to these diverse pressures, a strong environmental impact is expected in the North Channel of the Sado Estuary, particularly near Lisnave and Eurominas industries. In this area the type of contaminants discharged are diverse and more persistent, the hydrodynamics is lower, and additional contamination coming from Águas de Moura Channel can settle due to residual flow (hydrodynamics according to Neves, 1985). Spatial pattern evaluation of the fishing communities is not possible due to lack of data or difficulty in defining specific fish habitats inside the estuary. Nevertheless fishing activities are also an important pressure on the estuary, where for example some vulnerable or endangered species are included in the commercial caught species. Pollution on the estuary can cause a decrease in the quality of these resources and thus on the fishing local economy. The new wastewater treatment plant will treat wastewater corresponding to 300000 inhabitants-equivalent, including industrial and domestic effluents. It is expected, therefore, that some of these pressures, although high at the moment, will decrease in the near future.

No considerable advantages were noticed in the division of *Driving forces* and *Pressures* categories, after their quantification and spatial representation. The *Driving forces* indicators help to represent and list the human activities that are responsible by the *Pressures* and in some cases due to the lack of data some *Pressures* were only evaluated as *Driving forces*. Also, the indicators belonging to *Driving forces* category allow the distinction between positive or negative impacts on sustainable development, as is often the case with social and economic and institutional indicators (UN 1996, UN 2001). Moreover the gain in precision does not compensate the use of that category. We think that in future developments only the *Pressure* indicators need to be quantified, though considering encompassing the human activities, processes and patterns that impact on sustainable development.

Further work includes more detailed spatial analysis of those categories and the integration in the GIS of the remaining DPSIR indicators, and the different possible links between them.

This will allow the assessment of environmental conditions, a better integration with existing projects, programs, plans and policies, and the design of specific restoration/management actions for the Sado Estuary.

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PART V

SEDIMENT QUALITY ASSESSMENT

CHAPTER 7 – OPTIMIZATION OF AN ESTUARINE MONITORING PROGRAM: SELECTING THE BEST SPATIAL DISTRIBUTION

OPTIMIZATION OF AN ESTUARINE MONITORING PROGRAM: SELECTING THE BEST SPATIAL DISTRIBUTION

Caeiro, S., Nunes, L., Goovaerts, P., Costa, M. H., Cunha, M. C., Painho, M., Ribeiro, L. (2004). A. Soares, J. Gomez-Hernandez, and R. Froidevaux, (Ed.) *geoENV IV Geostatistical for Environmental Applications* Kluwer Academic Press. Dordrecht, pp. 355 - 366.

ABSTRACT

Estuarine monitoring programs are fundamental to evaluate pollution abatement actions, fulfillment of environmental quality standards and compliance with permit conditions. Their sampling designs should provide statistically unbiased estimates of the status and trends with quantitative confidence limits on spatial scale. The aim of this work is to select a subset of monitoring sampling stations based on locations from an extensive sediment campaign (153 sites) in the Sado estuary (Portugal). In each location three sediment parameters were determined with the objective of defining spatially homogenous environmental areas. The new monitoring program is based on fewer and on the most representative monitoring stations inside each homogeneous environmental area for their future contaminant assessment. Simulated annealing was used to iteratively improve on the mean square error of estimation, by removing one station at a time and estimating it by indicator kriging using the remaining stations in the sub-set, within a controlled non-exhaustive looping scheme. Different sub-set cardinalities were tested in order to determine the optimal cost-benefit relationship between the number of stations and monitoring costs. The model results indicate a 60 station design to be optimal, but 17 additional stations were added based on expert criteria of proximity to point sources and characterization of all homogenous areas.

KEY WORDS: Optimization, monitoring sampling, indicator kriging, estuarine sediments.

7.1 INTRODUCTION

Estuaries are coastal transitional water bodies with natural resources of high preservation values, providing important habitats for different species of organisms. The uses inside the estuary and around it have impacts on the water and sediment quality that may put at risk the equilibrium of the ecosystem. Environmental management of these ecosystems cannot be conducted effectively without reliable information on changes in the environment and on the causes of those changes. Ecological monitoring programs can represent an important source of that information. However, many of the existing programs are not effective. To assure effectiveness, monitoring programs should be designed to enable the statistical analysis and interpretation needed to relate cause and effects (Olsen *et al.*, 1999, Vos *et al.*, 2000).

The reliability of the sampling design depends on such a large degree on the sampling spatial distribution and size that their importance should not be underestimated (Haining, 1990). One or more of the following principles could govern the size of the sample (Cochran 1977; Clark and Hosking 1986; Strobel *et al.*, 2000): i) the required sampling size can be found if we have reasonable estimates of the population variance measured by a preliminary pilot survey; ii) certain statistical tests require a reasonable sample size; although no fixed minimum can be stated, a sample size of at least 30 is usually employed; iii) too large number of samples implies a waste of resources, and too small number diminishes the utility of the results; iv) finance and time may dictate a certain maximum number of samples.

In ecosystems like estuaries the spatial variability of key ecological indicators could be a measure to determine the appropriate monitoring sampling design (Strobel *et al.*, 2000).

The kriging interpolation is very useful to minimise the estimation variance for any fixed sampling design. The plot of the maximum value of the minimised estimation variance against sampling interval, or sample size, can be used to select sample size to achieve a required level of precision (Haining, 1990). For operational, economic or political reasons sometimes sampling sites for monitoring must be reduced and resource allocation optimized (Cochran, 1977). Optimal sampling scheme can then be designed by deleting sites from a current network so as to minimize the variance of estimation error, which means deleting the site that can be predicted best from the remaining sites (Cressie, 1993). Clever search algorithms like simulated annealing can then help designing the best sampling scheme. Difficulties usually arise in finding an optimal sampling plan and optimal kriging weights. Sampling plans can be important factors when looking for optimal spatial designs. Using the mean-squared prediction error of predictors, the rate of convergence to zero is faster for stratified random sampling than random or systematic random sampling designs (Cressie, 1993).

The sampling optimality criteria should not only be statistical but also cost related or economical (Cochran, 1977, Cressie, 1993, Vos *et al*, 2000). Sampling and parameters measurement costs are very important limitations and should be taken into account in the optimization procedure.

The aim of this work is to select, due to budget constrains, a subset of monitoring stations from an extensive stratified random campaign of estuarine sediments. This subset will be used to assess Sado Estuary sediment contamination in management units previously delineated. Spatial simulated annealing was used to optimize the sample locations. This information will be integrated in an environmental management system for Sado Estuary.

7.2 CASE STUDY

The Sado Estuary, located in the West Coast of Portugal, is the second largest in Portugal with an area of approximately 24,000 ha. The estuary comprises the Northern and the Southern Channels, partially separated by intertidal sandbanks. Most of the water exchange is made through the southern Channel. The estuary is linked to the ocean by a narrow and deep channel that makes a major contribution to the general pattern of the estuarine circulation (Neves, 1986). Most of the estuary is classified as a Nature Reserve. There are many industries mainly on the northern margin of the estuary. Furthermore the harbour associated activities and the city of Setúbal along with the mines on the Sado watershed also releases contaminants into the estuary. In other areas around the estuary, intensive farming, mostly rice fields, is the main land use together with traditional salt-pans and increasingly intensive fish farms. Most of these activities have negative impacts on water, sediment and biotic communities namely because they discharge to the estuary contaminants like heavy metals, or organic compounds (Caeiro *et al.*, 2002).

7.3 METHODS

7.3.1 Sediment homogenous areas delineation

In a first extensive campaign 153 sediment locations were sampled for analysis of properties of general characterisation: fine fraction (FF), organic matter (TOM), and redox potential (Eh). These key ecological parameters explain main variations in the type and behaviour of benthic organisms as well as contaminant mobility/accumulation (Rodrigues and Quintino, 1993). One method of determining sample size for multiple parameters assessment, is to specify margin error for the items that are regarded as most vital to the survey (Cochran, 1977). A systematic unaligned sampling design with a grid size equal to 0.365 km^2 was used based on prior information on the spatial variation of sediment granulometry (Fig. 7.1) (Caeiro *et al.*, 2003b – see Chapter 3).

This extensive campaign was intended to help defining homogeneous areas (future management units) for Sado Estuary within which contamination would be monitored using smaller sample sets.

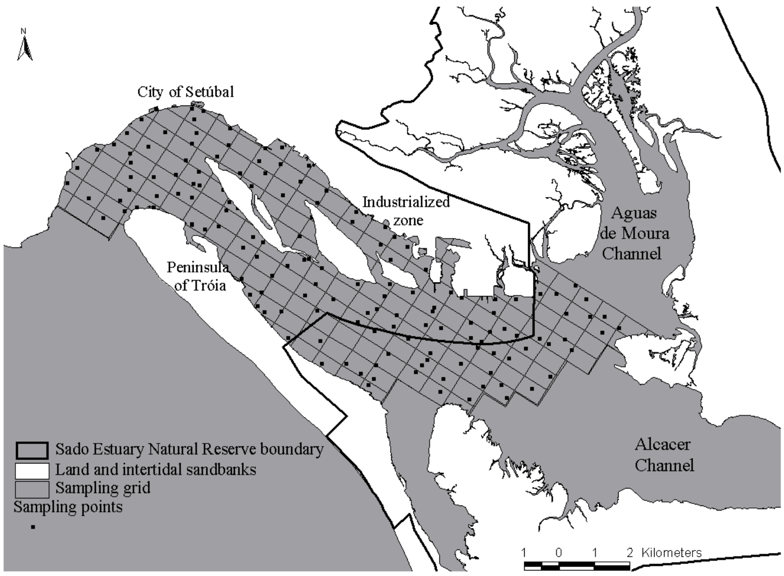


Figure 7.1 – Sado Estuary sediment sampling design (Adapted from Caeiro et al., 2003b).

These homogenous areas were delineated in 5 steps based on grouping individual sampling sites that have similar physicochemical properties while being geographically close (Caeiro *et al.*, 2003a – Chapter 4): 1) Principal component (PC) extraction of the 3 sediment properties variability (FF, TOM and Eh); 2) Variogram fitting of a spherical model to 1st PC factor scores; 3) Dissimilarity matrix determination; 4) Cluster analysis using the complete linkage rule on the dissimilarity matrix to estimate the probability of occurrence of four selected clusters at sampled stations; 5) Indicator kriging to interpolate these probabilities at unsampled stations; 6) Maximum likelihood classification of these unsampled stations.

The dissimilarity between any two sampling sites *i* and *j* (step 3) was computed following Oliver and Webster (1989) equation with spherical model adjustment (Goovaerts, 1997) to take into account the form of spatial variation. Step 5, started with an indicator,i, coding of classification results (x_α) at each sampled station x_α:

$$i(x_\alpha; z_l) = \begin{cases} 1 & \text{if} \quad z(x_\alpha) = z_l \\ 0 & \text{otherwise} \end{cases} \quad l=1,\dots,L \qquad \text{(eq. 7.1)}$$

where L is the number of clusters (four selected). For each cluster z_l, experimental indicator variograms are then computed and modelled:

$$\gamma(h; z_l) = \frac{1}{2N(h)} \times \sum_{\alpha=1}^{N(h)} \left[i(x_\alpha; z_l) - i(x_\alpha + h; z_l) \right]^2 \qquad \text{(eq. 7.2)}$$

The probability of occurrence of the l-th cluster at the unsampled station x is estimated as a linear combination of indicator data:

$$\hat{p}(x; z_l \mid B) = \sum_{\alpha=1}^{n_c} \lambda(x_\alpha; z_l) \times i(x_\alpha; z_l) \qquad \text{(eq. 7.3)}$$

where B is the set of n_c surrounding data $\{z(u_\alpha), \alpha=1,\dots, n_c\}$. The weights $\lambda(x_\alpha;z_l)$ are solutions of an indicator kriging system and account for data configuration and spatial continuity of clusters as modelled by indicator variograms. In theory, indicator cokriging estimator is better than the indicator kriging estimator because it accounts for additional information available across categories. However, indicator cokriging improves little over indicator kriging according to Goovaerts (1994).

7.3.2 Optimization model

The stations that produce the lowest estimation error variance, estimated using cross-validation technique (Deutsch and Journel, 1998), result in a spatial distribution with the highest accuracy. The objective function considers a set, S, of all the original stations, with cardinality Ω, and take a subset, S', with cardinality ω, such that $\omega < \Omega$.

Minimize:

$$s_{fp}^2 = \frac{1}{\omega} \sum_{\alpha=1}^{\omega} \left[i(x_\alpha; z_l) - i^*(x_\alpha; z_l) \right]^2, \omega \in S', S' \subset S \qquad \text{(eq. 7.4)}$$

Subject to:

$$\Psi_{S'}(A; z_l) \approx \Psi_S(A; z_l) \qquad \text{(eq. 7.5)}$$

s^2_{fp} is the mean squared error of estimation and equal to the variance of the estimation error if zero mean estimation errors are considered (i.e. no bias). $i^*(x_\alpha,z_l)$ is the indicator kriging estimated value, $\psi_S(A,z_l)$ and $\psi_{S'}(A,z_l)$ are the marginal probabilities of finding stations with values in $]z_{l-1}, z_l]$ in the original data set and in the candidate solution, respectively.

The new design *S'* must reflect the sediment physical and chemical variability detected with the prior sampling campaign. Therefore we imposed the constraint that the proportions of monitoring stations in each of the identified management units are similar to the proportions in the original sampling campaign (Table 7.1). Van Groenigen *et al.* (2000) also successfully used sampling constraints in spatial simulated annealing to optimise sampling scheme. The condition is not equality because, for practical computation, floating-point variables equality is machine dependent and varies with the precision. Instead, $\Psi_{S'}(A,z_l)$ may be bounded, and the constraint becomes:

$$\Psi_S(A;z_l)(1-\delta) \le \Psi_{S'}(A;z_l) \le \Psi_S(A;z_l)(1+\delta) \qquad \text{(eq. 7.6)}$$

A conditioning on the objective function with $\delta = 0.3$ was imposed. This condition is necessary to correct the bias introduced by variogram models fitting errors (when adjusting the theoretical models to the experimental variogram). If no conditioning is used increasing the number of stations will result in higher estimation error variances. This is due to the fact that at very low ω only stations with low estimation error in the optimal solution are included; as ω increases higher estimation error stations are included (Nunes, 2003).

Simulated Annealing (SA) algorithm with the Metropolis iterative improvement procedure (Metropolis *et al.*, 1953) was then used to solve the optimisation model. This procedure generalises by incorporating controlled uphill steps (to worse solutions). The procedure states the following: consider one small random change in the system at a certain temperature (the control parameters *t* is usually termed temperature); the change in the objective function is ΔOF; if $\Delta OF \le 0$, then the change in the system is accepted and the new configuration is used as the starting point in the next step; if $\Delta OF > 0$ then the probability that the change is accepted is determined by $P(\Delta OF) = exp(-\Delta OF/t)$; a random number uniformly distributed in the interval (0,1) is taken and compared with the former probability; if this number is lower than $P(\Delta OF)$ then the change is accepted. The SA algorithm runs in the following way: i) the system is *melted* at a high temperature (initial temperature, t_1); ii) the temperature is decreased gradually until the system *freezes* (no further OF change occurs); iii) at each iteration the Metropolis procedure is applied; iv) if any of the stopping criteria is reached the algorithm is stopped and the best solution found is presented. The generic SA algorithm for a minimisation, considering a neighbourhood structure *N*, a current solution *X*, a best solution found so far X_{best}, a solution space χ, a α temperature decrease control parameter and an objective function OF has the following pseudo-code:

```
Select an initial solution X_best;
Select an initial temperature t_1>0;
Select a temperature reduction factor;
Repeat
  Repeat
    Randomly select X∈ N(X_best);
     ΔOF = OF(X) – OF(X_best);
     IF ΔOF<0 then
       X_best = X
        else
     generate random z uniformly in (0,1);
          if z < exp(-ΔOF/t) then X_best = X;
  Until iterations = max_iterations
  Set t = αt;
Until stopping condition = true;
X_best is the optimal solution found.
```

In order to speed-up the process several improvements have been proposed, namely by limiting the number of iterations at each temperature, i.e., defining the number *max_iterations*. The dimension of the Markov chain has been proposed to be a function of the dimension of the problem (Kirkpatrick *et al.*, 1983): temperature is maintained until 100Ω solutions (iterations), or 10Ω successful solutions have been tested, whichever comes first. Ω stands for the number of variables (stations) in a problem.

A specific computer code in FORTRAN that incorporates both the estimation error variance and the SA algorithm was developed by (Nunes, 2003) to optimise location problems and adapted to this specific problem. Runs were made on PC Intel 2000 MHz machines.

Fourteen different monitoring network dimensions (cardinality of *S'*: ω) were tested, {25,30,35,40,45,50,60,70,80,90,100,110,120,130} according to the following scheme: i) impose a number of monitoring stations (ω) to be included in the new design; ii) find the optimal allocation solution with SA; iii) increase ω and return to i). SA solutions are considered optimal when more than 70% out of 20 consecutive runs with the same objective function conditions (ω, δ) and SA parameters have the lowest and equal s_{fp}^2 value.

A complementary analysis comparing the loss in accuracy versus reduction in exploration costs as stations are removed was also performed. For that purpose a cost per sampling was computed based on the previous sampling campaign and laboratory analysis costs (official costs of the laboratory where the analysis are going to be made - ControLab, lda.): i) linear distance between *n* sampling point: *n*/study area (56 km^2); ii) boat velocity: 12,8 km/h; iii) hours of work per day: 7 h/day; iv) time for sampling: 20 min; v) Boat cost per day: 250 Euros; vi) cost per total contaminant analysis: 500 Euros (discount: 25 % from 20 to 50 stations, 30 % from 55 to 100 stations and 40 % from 105 to 135 stations).

7.4 RESULTS AND DISCUSSION

Table 7.1 lists four different physical and chemical management units (clusters) based on the sampling campaign data and results from hierarchical classification (step 4), and their frequencies in the study area.

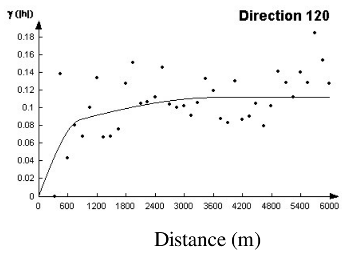
For each cluster, the indicator variogram was computed along four directions and a geometric anisotropic spherical model was fitted (Fig. 7.2 and see Chapter 4).

Fig. 7.3 shows the spatial accuracy plotted versus the monitoring network dimension. Beyond 60, each new added station had little effect on the monitoring spatial accuracy (s_{fp}^2). Sixty is therefore considered as the optimal ω value. The resulting network was overlaid on the sediment homogenous areas within the estuary coastline (Caeiro *et al.*, 2003b – Chapter 3) using Arcview/arcinfo 3.2 GIS software (Fig. 7.4a). In cluster one and two (z_1 and z_2) the estimation errors are higher, therefore leading the optimisation algorithm to select preferentially the two remaining clusters with lower estimation errors. These clusters are therefore more densely sampled than in the original data set, as a way to compensate for the bias introduced. Also when high or low values of a cluster are grouped in small areas scattered in the study area, their relative frequencies are low or data values is too random, the variogram fitting becomes difficult and prone to error. The result is the fitting of theoretical variograms that only roughly approximate the real variability and large estimation errors. This does not hinder the geostatistical method, but justifies the need to impose reproduction of the original proportions (Nunes, 2003).

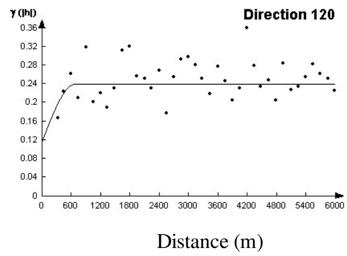
Table 7.1 – Physical and chemical parameters of each cluster (average and standard deviation values) and their frequency.

	Clusters (s)			
Sediment Parameter	High organic load (z_1)	Medium high organic load (z_2)	Medium organic load (z_3)	Low organic load (z_4)
TOM (%)	8.6 ± 2.4	4.2 ± 1.4	1.9 ± 0.7	0.9 ± 0.3
FF (%)	60.4 ± 27	21.7 ± 11.8	9.1 ± 7.8	1.5 ± 1.3
Eh (mV)	-278.9 ± 68.6	-178.8 ± 72.6	-137.4 ± 50.9	74.4 ± 49
Freq. (%)	11.76	37.91	23.53	26.80

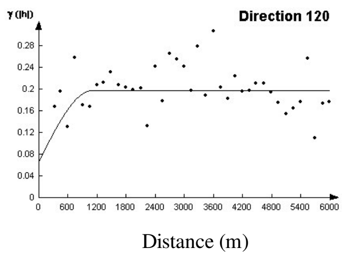
CLUSTER 1
c_0 = 0.002;
c_1= 0.073, a_{1max} = 854, a_{1min} = 769
c_2= 0.038, a_2 = 3721



CLUSTER 2
c_0 = 0.117;
c= 0.123, a_{max} = 671, a_{min} = 201



CLUSTER 3
c_0 = 0.068
c= 0.130, a_{max} = 1098, a_{min} = 1043



CLUSTER 4
c_0 = 0.092;
c_1= 0.07, a_{1max} = 1520, a_{1min} = 1034
c_2= 0.04, a_{2max} = 2135, a_{2min} = 1772

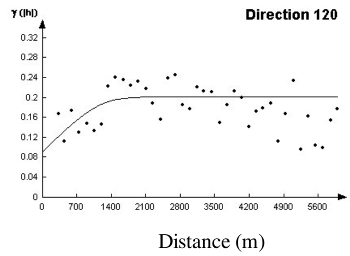


Figure 7.2 – Cluster experimental directional variograms and spherical model fitted for 120º, the major direction of anisotropy. Other directions (not shown) included 30º, 75˚ and 165º.

Figure 7.4a) indicates that not all the homogenous areas are sampled in the optimal scheme solution, in particular areas belonging to clusters with high organic load (1 and 2), for the reasons explained earlier. Most of these cluster 1 and 2 areas are near contaminant point sources, mainly in the North Channel. Thus 17 stations were added to the optimal ω value according to expert knowledge aiming to characterize the impact of those point sources and homogenous areas not included in the optimised network (Fig. 7.4b).

The number of stations to evaluate contamination in the study area (77 stations/56 km^2, corresponding to 1.38 stations/km^2) is within the average of sediment sample size of Environment Monitoring Assessment Program (EMAP) of United States Environmental Protection Agency (USEPA) for small estuaries. The sample sizes for the different estuaries of EMAP vary from 0.11 to 4.16 stations/km^2 (Strobel *et al.*, 2000). Such a wide interval might be related to the spatial variability of sediment parameters in each coastal zone, which is caused by differences related to geomorphological, biological and human pressures.

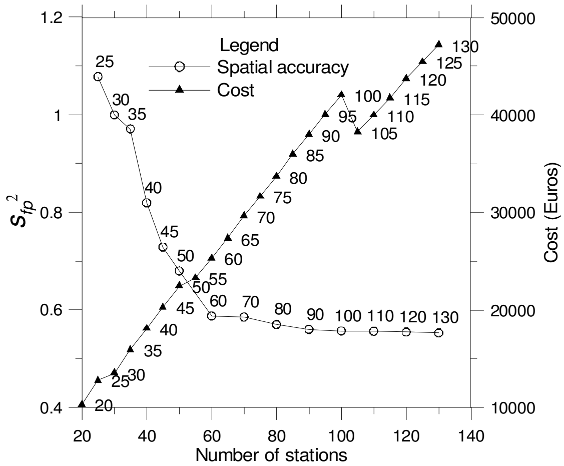


Figure 7.3 – Estimation error variance and cost versus number of monitoring stations.

The exploration costs analysis (Fig. 7.3) showed that costs are always increasing and only for large number of stations (from 110 to 115) does the cost decrease. Indeed the cost of contamination concentration analyses has a high weight in the total cost and only for 105 laboratory analysis does the laboratory discount significantly affect the total cost.

Although seventy-seven stations still represent a high cost (about 60 % of stations total number cost), this budget figure is considered necessary at the present time for a contamination assessment. For any future long-term monitoring program to assess estuary ecological condition, a lower number of sampling sites could be chosen. Thirty sampling stations should represent a good number for a monitoring program since: i) each of the 19 management units could be sampled at least at one location or two in case of larger areas, ii) it is a statistical minimum required; iii) the cost is not too high (and similar to 25 stations – see

Fig. 7.3). Nevertheless, 30 stations will represent about 40 % loss in spatial accuracy, compared to the 60 stations obtained by the model (see Fig. 7.3).

In the future developments for a monitoring program of the environmental management system of the estuary, the model should take into account two strata in the study area. One in the North Channel near pollution sources and the other in the South where the hydrodynamics is highest and the pollution sources are non-point. Vos *et al.*, (2000) discuss that the identification of relevant subsystems or strata for monitoring purpose, is very important to maximise diagnostic of ecological changes. In these strata changes in the anthropogenic inputs or “controlled variables” are expected. Also, once contaminants have been measured at the 77 sampling points a new optimisation criterion could be developed to sample preferentially areas with high priority (e.g. high concentrations). Van Groenigen *et al.* (2000) used a spatial weight function in spatial simulated annealing that allows distinguishing between areas with different contamination priorities. This could be achieved through Weighted Mean of Shortest Distance; i.e. the fitness is extended with a location-dependent weighing function, or/and using probability maps of contamination and indicator kriging. In particular in our case the weight function should take into account small areas and distance to contaminant sources.

a) b)

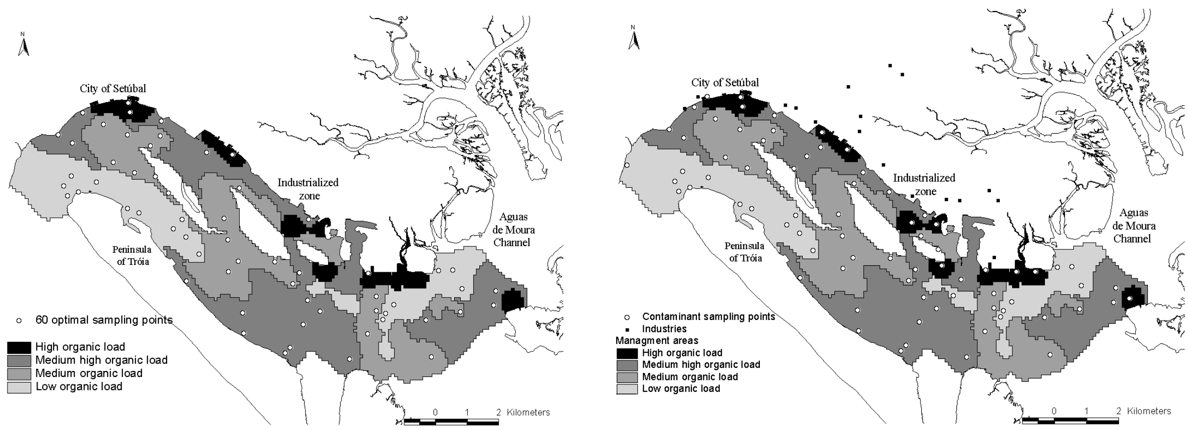


Figure 7.4 – Monitoring networks a) for ω value = 60 stations; b) with 60 optimal stations and additional expertise criteria (17) (Location of industries from Araujo *et al.* (2003).

7.5 CONCLUSIONS

Monitoring programs should be planned in order to provide quantitative and scientific assessments of pollutants’ complex effects on these systems. Optimal sampling designs for ecological condition assessment should take into account not only statistical criteria but also historical knowledge about the study area. In particular estuaries have always areas with different priorities (e.g. human pressures or more sensitive areas). From an extensive campaign including 153 sampling points, a sampling design with 77 stations was selected for sediment contaminant assessment in Sado estuary. This selection was based on minimization of indicator kriging mean square error estimation and expertise knowledge. For a future long–term monitoring program of the estuary condition assessment a reduced subset of 30 stations should be chosen based on definition of contaminant priority areas.

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CHAPTER 8 – ASSESSING SEDIMENT HEAVY METALS CONTAMINATION IN THE SADO ESTUARY: AN INDEX ANALYSIS APPROACH

ASSESSING SEDIMENT HEAVY METALS CONTAMINATION IN THE SADO ESTUARY: AN INDEX ANALYSIS APPROACH

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(submitted to *Ecological Indicators*)

ABSTRACT

The Sado Estuary in Portugal is a good example where the human pressures and natural values occur and where global contamination has not been evaluated in an understandable way for managers. The aim of this work is to assess the sediment heavy metal contamination in this estuary using different types of metal assessment indices and spatial analysis tools like GIS and interpolation surfaces. Seventy eight stations were sampled along the main bay of the estuary, and a set of heavy metals and metalloids were determined, Cd, Cu, Pb, Cr, Hg, Al, Zn and As, as well as sediment fine fraction contents, organic matter and redox potential. Various contamination, background enrichment and ecological risk indices were used, tested and robustness evaluated. All heavy metals are strongly correlated, and the indices represent well heavy metals behavior. Difficulties arise for some indices when defining their boundaries (minimum and maximum) and when comparing with other estuaries, thus better methods of standardization should be a priority issue. According to the index that has the highest classification - Sediment Quality Guideline Quotient – only 3 % of the stations are highly contaminated and with high potential for observing adverse biological effects, but 47 % have moderate potential for observing adverse biological effects. The cadmium is the contaminant of higher concern, followed by Arsenic.

KEYWORDS: Heavy metals assessment, estuarine management, sediments, pollution, indices.

8.1 INTRODUCTION

Estuaries receive significant anthropogenic inputs from both point and non-point sources upstream and from metropolitan areas, tourism and industries located along estuarine edges.

Estuarine sediment contamination is receiving increasing attention from the scientific community, since it is recognized as a major source of stress to the ecosystem health (Chapman and Wang, 2001, Riba *et al.*, 2002b). Thus, the proper assessment of sediment contamination in estuaries and its biological and ecological significance is crucial.

Chemistry-based approaches for assessing sediment contamination are based on reliable measurements and interpretation of contaminant concentrations in the sediments. While the overlying water in estuaries can be heterogeneous because of different mixtures of fresh and saline water, a much higher degree of heterogeneity and variability exits within estuarine sediments also because of the diverse and complicated composition of the sediments. Hence any assessment approach based on sediment concentration needs to consider grain size effects, normalizing these relative to sediment contaminant concentration (Chapman, 1996). The normalization can be done using ratios, but this method although simple may be inappropriate when we are analysing sediments with different grain sizes (Ruiz, 2001). Regression line comparisons are the most appropriate approaches to analyse background enrichment chemical assessment (Chapman and Wang, 2001). Regression methods may be more powerful using less-absolute-values robust regression instead of least squares regression analysis (Grant and Middleton, 1998, Chapman and Wang, 2001). This approach does not require any careful examination of data and removal of outliers which involves an element of subjectivity and bias the results (Grant and Middleton, 1998).

For better management of estuarine ecosystems their contamination assessment should be easily communicated to the local managers and decision makers. Environmental quality indicators and indices are a powerful tool for processing, analyzing and conveying raw environmental information, to decision-makers, managers, technicians or the public (Ramos *et al.*, 2002). Their visualization through maps using a Geographical Information System turns their transmission even easier and more successful.

In the last decades different metal assessment indices applied to estuarine environments have been developed. Each one of them aggregates the metal contaminants concentration and/or compares the contaminants with: i) reference clean and/or polluted stations or simply with not any comparison, and can be named as <u>contamination indices</u>; ii) different baseline or background levels - <u>background enrichment indices;</u> iii) Sediment Quality Guidelines or Values -SQG - <u>ecological risk</u> indices. They also differ in the aggregation methods used.

Table 8.1 presents an overview of indices to assess contaminants based on their chronological evolution, their description and some comments and/or drawbacks.

When using summary indices, normalized for example to a reference value, substantial loss of information can occur during the conversion of multivariate data into single proportional indices, including spatial relational information. However, such indices have provided useful information in the past and continue to do so. Also it provides a single and highly visual data presentation, which can be explained to and understood by non-scientists (Chapman, 1996).

Sediment quality guidelines are very useful to screen sediment contamination by comparing sediment contaminant concentration with the corresponding SQG. These guidelines evaluate the degree to which sediment-associated chemical status might adversely affect aquatic organisms and are designed to assist sediment assessors and managers responsible for the interpretation of sediment quality (Wenning and Ingersoll, 2002). They have been largely developed for marine waters (e.g. Long *et al.*, 1995) but few have been specifically developed for estuarine waters (Chapman and Wang, 2001). Wilson and Jeffrey (1987) work is a rare example of SQG guidelines developed specifically for estuaries. Donze *et al.* (1990) listed background concentration for several estuaries in Europe and USA.

The Sado Estuary in Portugal is a good example where human pressures and natural values occur and where global degree of metal contamination has not been assessed also in an understandable way for managers. The aim of this work is to assess the heavy metal contamination in this estuary using different types of indices and compare and discuss them. In addition other tools like GIS and interpolation surfaces are used to assess metal contamination. These indices will be integrated with benthic and toxicity indices for sediment quality assessment. This Sediment quality will be represented in management units to be part of a management and data system for Sado Estuary. The management units were delineated based on sediment parameters like Total Organic Matter (TOM), Fine Fraction (FF) and redox potential (Caeiro *et al.*, 2003 – see Chapter 4).

Table 8.1 –Indices to assess contamination applied to estuarine environments.

Author	Index name: type	Description	Coments/drawbacks
Johanson & Johnson (1976) *fide* Ott (1978)	Pollution Index (*PI*): <u>Contamination index</u>	$PI = \sum_{i=1}^{n} W_i C_i$ (eq. 8.1) W_i – weight for pollution variable *i* C_i – highest concentration of pollution variable *i* reported in a location of interest. For each pollutant *i*, the weight was based on the reciprocal of the median of observed concentrations.	• This index allows the identification of priority contaminations sites for implementation of decontamination actions. It needs several measures in the same sampling location. No threshold classification from unpolluted to high pollution.
Hakanson (1980) Kwon and Lee (1998).	Degree of contamination (*DC*) (sub-index of an Ecological Risk Index): <u>Background enrichment index</u>	$DC = \sum_{i=1}^{n} C_f^i = \sum_{i=1}^{n} \frac{\overline{C}_{0-1}^i}{C_n^i}$ (eq. 8.2) C_f^i – contamination factor $\overline{C}_{0-1}^i$ – mean content of the substance in question (i) from superficial sediment (0-1 cm) from accumulation areas (at least 5 samples). C_n^i – the reference level (according to (Hakanson. L. 1980). DC< *n* (nº of contaminants) – low level of contamination; *n* < DC <2*n* – moderate degree of contamination; 2*n*<DC< 3*n* – considerable degree of contamination; DC> 3*n* very high degree of contamination	• It was developed and tested for lakes, although has already been successfully used for coastal areas (Kwon and Lee, 1998). It needs at least 5 samples, which provide an area cover of the study area. Only build for 8 contaminants (PCB, Hg, Cd, As, Cu, Pb, Cr).
Satsmadjis and Voutsinou-Taliadouri (1985)	Index of Metals Pollution in Marine Sediments (*q*): <u>Background enrichment index</u>	The assessment of the degree of pollution of sediment by a element requires at first the relation of its contents, *c*, to the granulometric composition of the substratum in a clean section of the investigated region, and the metal concentration estimation for no contaminated sediment is then evaluated on the basis of the grain size composition: $f = g + \frac{t}{0.2g+5}$ (eq. 8.3) $c = EKd^{\log f / \log 5}$ (eq. 8.4) $q = \frac{C'}{c}$ (eq. 8.5) *f* –clay equivalent *g* – percentages of clay *t* – percentages of silt c – metal concentration in clean section of the investigated region. *E* and *K* - constant. *d* – enrichment constant, expresses the magnitude of the influence of the grain size on the concentration of the metal. The enrichment induced by fine particles is very slight for $d < 1.2$, moderate for $1.2 \leq d < 1.4$, substantial for $1.4 \leq d < 2$ great for $2 \leq d < 4$ and huge for $d \geq 4$. *C'*- true concentration of the metal. If it exceeds 1, measures the extent of the pollution by the metal in question.	• Calculated based on data of one specific place – Greek gulfs. Not tested in other coastal ecosystems. According to the author it is difficulties to find the proper data to set up and to compute eq. 8.4, since not easily discernible factors may boot the level of an element in a seemingly virgin zone. It does not incorporate all metals into one value. It needs the separated measurement of silt and clay. No threshold for maximum pollution.

Table 8.1 –Indices to assess contamination applied to estuarine environments (cont).

Author	Index name: type	Description	Coments/drawbacks
Wilson and Jeffrey (1987)	Pollution Load Index (*PLI*): <u>Ecological risk index</u>	For each contaminant the PLI is calculated: $PLI = anti\,log_{10}\left(1-\frac{C-B}{T-B}\right)$ (eq. 8.6) *B* – Baseline value – not contaminated *T* – Threshold, minimum concentrations associated to degradation or changes on the quality of the estuarine system. Wilson and Jeffrey (1987), defines *B* and *T* for the different contaminant. *C* – Concentration of the pollutant. For each place the PLI is calculated taking into account all the *n* contaminants: $PLI = (PLI_1 \times PLI_2 \times ... \times PLI_n)^{\frac{1}{n}}$ (eq. 8.7) Varies from 10 (unpolluted) to 0 (high polluted).	• This index allows the comparison between several estuarine systems. Easy to implement. It has been applied successfully in European estuaries (Wilson *et al.* 1987; Wilson and Elkaim 1991; Ramos 1996), and US estuaries (Wilson, 2003). Ramos (1996), used this index with other aggregation methods like arithmetic average and minimum sub-index and obtained good results. Evaluate toxicity, since takes into account SQG comparison. Values of baseline and limiar not defined locally for each coastal zone analyzed and not revised lately.
Chapman (1990)	Index for chemistry (Ratio-to-Reference RTR) of the Sediment Quality Triad component (*I*): <u>Contamination index</u>	$I = \frac{\sum_{i=n} RTR_i}{n} \forall i$ (eq. 8.8) $RTR_i = \frac{v_i}{(v_i)_0}$ (eq. 8.9) n- total variable number v_i – value of each parameter *i* $(v_i)_0$ – value of each parameter at reference site.	• Useful in time-series monitoring, of summarizing changes by time and location. It needs reference site values. It could give imprecise values because they could be over influenced for one of the measures used in the final composite values (DelValls *et al.*, 1998b). No threshold for maximum pollution.
Usero *et al.* (1996)	Metal Pollution index (*MPI*): <u>Contamination index</u>	$MPI = (M_1 \times M_2 \times M_3 \times ...... \times M_n)^{\frac{1}{n}}$ (eq. 8.10) Where M_n is the concentration of metal *n* expresses in mg/kg of dry weight.	• Simple but do not compare the metal concentration with any baseline or guidelines. No threshold classification from unpolluted to high pollution.
DelValls *et al.* (1998b)	Index for chemistry (new Maximum RTR) of Sediment Quality Triad component (*NI*): <u>Contamination index</u>	$NI = \frac{\sum_{i=1}^{n} RTM_i}{\left(\sum_{i=1}^{n} RTM_i\right)_0} \forall i$ (eq. 8.11) $RTM_i = \frac{RTR_i}{(RTR-m_i)}$ (eq. 8.12) $(RTR - m_i)$ = RTR maximum value obtained for the parameters *i* $(..)_0$ – Reference site.	• The use of the maximum reference value (reference polluted station) to normalize a dataset from Sediment Quality Triad (SQT) permits the classification of each component variable between maximum and minimum. It needs reference site values. No threshold for maximum pollution, to compare with other ecosystems.
Long and MacDonald (1998)	Mean sediment quality guideline quotient (*SQG-Q*): <u>Ecological risk index</u>	Takes into account a complex mixture of contaminants in each location (NSTP-National Status and Trend Program): $SQG-Q = \frac{\sum_{i=1}^{n} PEL-Q_i}{n}$ (eq. 8.13) $PEL-Q = \frac{contaminant}{PEL}$ (eq. 8.14) *PEL-Q* – probable effect level quotient *PEL* – Probable effect level for each contaminant (concentration above which adverse effects frequently occur) (Macdonald *et al.*,1996). Sediment locations are then scored according to their impact level (MacDonald *et al.* 2000): $SQG\text{-}Q \leq 0.1$ unimpacted – lowest potential for observing adverse biological effects $0.1 < SQG\text{-}Q < 1$ moderate impact potential for observing adverse biological effects $SQG\text{-}Q \geq 1$ highly impacted potential for observing adverse biological effects.	• It mixtures in a same SQG all contaminants, including metals, PAH ou PCB. Evaluate toxicity, since take into account SQG comparison. It can also be used with other SQG like Effect Range Median (ERM) (Long *et al.*, 1995), or others. Other scores can be used instead of 1. MacDonald *et al.*, (2000) used threshold of 1 and 2.3 and obtained better results with 1.

Table 8.1 –Indices to assess contamination applied to estuarine environments (cont).

Author	Index name: type	Description	Coments/drawbacks
Ingersoll *et al.* (1999) *fide* MacDonald *et al.* (2000)	Mean sediment quality guideline quotient (*SQG-Q'*): Ecological risk index	Same procedure of earlier SQG-Q, but calculates the Quotient separately for each type of contaminant: Metals, PCBs and PAHs, than, the mean SQG-Q is calculated by determining the average of each SQG-Q type of contaminants (USEPA procedure). Sediment locations are scored in the same way as NSTP	• Evaluate toxicity, since it take into account SQG comparison. It can also be used with other SQG like ERM or scored with other thresholds.
Ferreira (2000)	Equation sub-index Sediment Quality (*EQUATION*): Ecological risk index	This sub-index is integrated in a Estuarine Quality index based on Key Physical and Biogeochemical Features. The sediment quality sub-index is evaluated through sediment contamination, bioaccumulation and biodiversity descriptors. The sediment contamination is evaluated in terms of area affected according to a probabilistic approach. The system is divided into a set of grid cells, and on contamination levels defined using the PEL. For each grid cell, the median value for each sampling station is determined and if any of the PEL values for indicator contaminants are exceeded, the stations is considered polluted. The contamination of a grid cell is based on the proportion of contaminated stations contained. Five grades are defined, ranging from light contamination (10% of area polluted) to gross pollution (> 70 % of area).	• According to the author the rate of changes of persistent pollutants in the sediment is usually low, eliminating the need for dedicated synoptic sampling. Only applicable for gross comparison between estuaries, not for detailed management of a particular system.
Fairey *et al.* (2001)	Mean sediment quality guideline quotient as indicator of contamination and acute toxicity (*SQG-Q1*): Ecological risk index	$SQG-Q1=\left(\left(\frac{\left[\frac{Cd}{4.21}\right]+\left[\frac{Cu}{270}\right]+\left[\frac{Pb}{112.18}\right]+\left[\frac{Ag}{1.77}\right]+\left[\frac{Zn}{410}\right]+\left[\frac{TChlordane}{6}\right]+\left[\frac{dieldrin}{8}\right]+\left[\frac{TPAH_{OC}}{1800}\right]+\left[\frac{TPCB}{400}\right]}{9}\right)\right)$ (eq. 8.15) The constant values correspond to PEL, in the case of Cd, Ag, Pb, ERM in case of Cu, Zn, total chlordane and Dieldrin, consensus guideline defined by Swartz (1999) *fide* Fairey *et al.* (2001) for total PAH and consensus guideline defined by MacDonald *et al.* (2000) *fide* Fairey *et al.* (2001) for total PCB. Sediments have a high probability of being toxic to amphipods when SQG-Q1 is high (> 1.5) and a low probability of being toxic when SQGQ1 is low (<0.5).	• It is meant to serve only as a central tendency indicator. It minimizes the potential for impact from any one component. It is prudent to consider chemical exposure on an individual chemical basis in addition to the chemical matrix basis described here. SQG-Q1 ranges are themselves currently subject to investigation. It is only focus on acute toxicity of sediment to marine amphipods as the sole measure of biological response.
Ruiz (2001)	New Index of geoaccumulation (Ni_{geo}): Background enrichment index	$NI_{geo}=log_2\frac{C_n}{1.5\times B_n}$ (eq. 8.16) B_n – concentration of the metal *n* in unpolluted sediments, according to a list of regional backgrounds for the different grain sizes (Medium sand, Fine sand or Silt and Clay) C_n – concentration of the metal. NI_{geo}<1 very low polluted; 1< NI_{geo} <2 low polluted; 2< NI_{geo} <3 moderate polluted; 3< NI_{geo} <4 high polluted; NI_{geo} > 5 very high polluted.	• First version of this Index was developed for rivers by Muller (1981) *fide* Ruiz (2001), but this new version was applied in estuaries. It needs a grain size classification of the sediment. Have a great advantage of using a different background level depending on sediment grain size. B_n only developed for Cr, Cu, Zn and Pb. It does not aggregate all metals into one value.
Shin and Lam (2001)	Marine Sediment Pollution Index (*MSPI*): Contamination index	$MSPI=\left(\sum_{i=1}^{n}q_iw_i\right)^2/100$ (eq. 8.17) q_i – sediment quality rating of the *i* contaminant w_i - weight attributed to the *i* variable (proportion of eigenvalues obtained from the results of a Principal Component Analysis (PCA). For each variable the sediment quality is rated (q_i) based on the percentile in the data set: MSPI 0-20 –sediment excellent conditions; MSPI 21-40 –sediment good conditions; MSPI 41-60 –sediment average conditions; MSPI 61-80 –sediment poor conditions; MSPI 81-100 –sediment bad conditions. The index is also scored with this scale.	• Site-specific turning the index more accurate. It has a complex computation (PCA development). This index shown significant correlation with benthic and toxicity data.

Table 8.1 –Indices to assess contamination applied to estuarine environments (cont).

Author	Index name: type	Description	Coments/drawbacks
Riba *et al.* (2002a)	Metal enrichment index (*SEF*): Background enrichment index	$SEF = \frac{C_i - C_0}{C_0}$ (eq. 8.18) C_i- total concentration of each metal i measured in the sediment. C_0 – heavy metal background level established for the studied ecosystem.	• It does not aggregate all metals into one value. No threshold for maximum pollution.
Riba *et al.* (2002a)	Potential ecological risk index (*ERF*): Ecological risk index	$ERF = \frac{C_i - C_{SQV}}{C_{SQV}}$ (eq. 8.19) C_i- total concentration of each metal measured in the sediment C_{SQV} – highest concentration of the heavy metal non-associated with biological effects (chemical concentration associated with adverse effects) – sediment quality values reported by DelValls and Chapman (1998). Polluted stations have values equal or higher than 1.	• It does not aggregate all metals into one value. It uses site-specific sediment quality guidelines.

8.2 METHODS

8.2.1 Study area

The Sado Estuary is the second largest in Portugal with an area of approximately 24,000 ha. It is located in the West Coast of Portugal. Most of the estuary is classified as a Natural Reserve but also with an important role in the local and national economy. There are many industries mainly on the northern margin of the estuary. The most polluting industries are the pulp and paper, pesticides, fertilizers, ferments, food and shipyard (Catarino *et al.*, 1987). Furthermore the harbor-associated activities and the city of Setúbal along with the copper mines on the Sado watershed use the estuary for waste disposal purpose without suitable treatment. In other areas around the estuary intensive farming, mostly rice fields, is the main land use together with traditional salt-pans and increasingly intensive fish farms.

The Sado Estuary is characterized by a North Channel with weaker residual currents flow and shear stress, that enhance accumulation of sediment allowing locally introduced pollutants settle down rather than to be carried away. The southern channel, separated by the North Channel by sandbanks, is highly dynamic with tides being mainly responsible for water circulation. Geometric characteristics distinguish the outer estuary (our study area) from the inner estuary, corresponding to a narrow channel (Alcacel Channel). The inner part of the outer estuary (entrances of Águas de Moura and Alcácer Channels) is quite shallow with tidal flats (Neves, 1985).

8.2.2 Sampling design and analytical procedures

Seventy eight stations were sampled in the outer Sado Estuary between October of 2000 and January of 2001 (Fig. 8.1). The sampling design was chosen to assess the sediment quality of management units previously delineated (Caeiro *et al.*, 2004 – Chapter 7). A set of heavy metals total concentrations (Cd, Cu, Pb, Cr, Hg, Al, Zn) and metalloid (As), were determined. Accurately weighted aliquots of about 1 g of sediment were digested according to the methods USEPA (1996). The analytical technique used was Inductively Coupled Plasma Atomic Emission Spectroscopy (ICP-AES). In the case of Mercury a CMA (Concomitant Metals Analyser) system was used in the ICP-AES for a detection limit improvement. Certified reference material and spiked samples were used to evaluate the accuracy of the analytical methods. Total Organic Matter (TOM), sediment Fine Fraction (FF) and Redox Potential (Eh) were also determined for each location (Caeiro *et al.*, 2003 – Chapter 4).

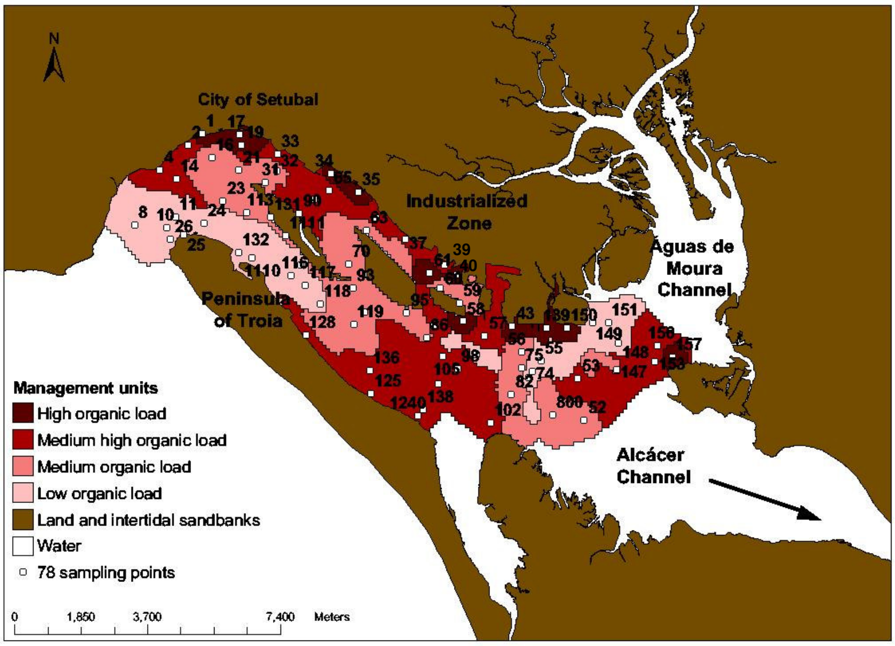

Figure 8.1 – Location of the sampling points in Sado Estuary and the management units. These areas are divided in four groups according to their organic load (Adapted from Caeiro *et al.*, 2003).

8.2.3 Background enrichment per contaminant

To evaluate the background contamination, the heavy metals concentrations were normalized using Robust Regression (using least absolute values) analysis on fine fraction contents. FF was the parameter strongest correlated with the studied metals (R^2 varied from 0.57 in Pb to 0.95 on Cr metals) compared to TOM and Al which are other most common parameters used as metal normalization factors (Luoma, 1990). For the regression no data transformation was computed. Nevertheless, some researchers have used log-transformed metals concentration in the regression analyses (e.g. Summers *et al.*, 1996). Such transformations do not improve correlation of the metals-sediment constituent concentrations of the data set. Furthermore, linear regression provides direct correlation with the physical mixing and geochemical factors which affect the overall concentration of metals in sediments. This correlation is lost when metal concentrations are transformed (Strobel *et al.*, 1995). Given that, for index calculation and comparison with sediment guidelines or baseline levels the metals original concentrations are needed, no normalization was used for that case. Data transformation was only performed for interpolation surfaces and multivariate analyses like Principal Component Analysis (PCA) and hierarchical analysis, after normality testing. When necessary log(x+c), c – lowest non-zero value found for each metal, was then computed (Chapman, 1996).

Since a more densely sampled dataset for the same study area and time period is available (153 sampling points - Caeiro *et al.*, 2003 – Chapter 4), interpolation using co-kriging was computed for each heavy metal spatial results interpretation. Sediment FF was used as a secondary variable. Co-kriging helps to reduce the variance of the estimation errors where the cross-correlation between variables are exploited and where the primary variable of interest is undersampled (Isaaks and Srivastava, 1989).

8.2.4 Indices calculation

The indices were chosen (from Table 8.1) whenever input data was available, all contaminants were integrated in one value and the most similar ones were rejected (Table 8.2): PIN, DC (eq. 8.2), PLI (eq. 8.6 and eq. 8.7), I (eqs. 8.8 and 8.9), MPI (eq. 8.10), NI (eqs. 8.11 and 8.12), SQG-Q (eqs. 8.13 and 8.14), and MSPI (eq. 8.17). A new Pollution Index, PIN, was adapted from PI (eq. 8.1), based on the Portuguese law of dredge materials classification (DR, 1995):

$$PIN = \sum_{i=1}^{n} \frac{W_i^{\,2} C_i}{B_{1i}} \qquad \text{(eq.8. 20)}$$

Where:
W_i- class of the contaminant *i* considering their contamination degree (from 1 to 5)
C_i- concentration of the contaminant *i*
B_{1i}-Concentration of contaminant *i* in Class 1 (baseline value).

According to that law the sediments (and the Index) can be classified in 5 categories from clean to highly contaminated sediments (Table 8.3). *PIN* values were normalized in nominal scale from 1 to 5 according to the threshold classification values. Each index threshold was calculated using the value of W_i and C_i of the corresponding class: Class 1: [0 –7[; Class 2: [7 – 95.1[; class 3: [95.1–518.1[; class 4: [518.1–2548.6[class 5: [2548.6– ∞[.

For DC calculation one value of each contaminant per sampling station was used and not five samples per each area, according to the original index, due to lack of data.

For the indices I and NI, stations inside the management area at the entrance of the estuary were chosen as the reference stations (8, 10, 11, 24, 25, 26, 111, 116, 117, 118, 132, 1110)

(Fig.8.1). The concentration values of each metal in the reference site were calculated using the median values of these 12 stations. This area has high hydrodynamics and has no direct influence of any anthropogenic source. The baseline concentrations of the heavy metals found in these stations are in accordance or even lower compared to earlier works done in the Sado Estuary clean areas (e.g. Quevauviller *et al.*, 1989, Quintino, 1993). ANOVA test was used to test differences between reference sites and the other stations (Chapman, 1996), after normality assumptions tested. A cluster analysis was also computed (tree clustering), using the seven studied heavy metals, As, Eh, FF and TOM, to confirm if the reference stations were grouped together.

Table 8.2 – Index calculated in this study and guidelines used.

		Guidelines (mg/kg)							
Indice	**Classification**	**Cd**	**Pb**	**Zn**	**Cu**	**As**	**Cr**	**Hg**	**TOM**
New Pollution Index (PIN)	Clean sediments (DR, 1995)	1	50	100	35	20	50	0.5	-
Degree of Contamination (DC)	Pre-industrial reference level (Hakanson, 1980)	1	70	175	50	15	90	0.25	-
Pollution Load Index (PLI)	Baseline (Wilson and Jeffrey, 1987)	0.5	10	20	5	5	5	0.05	1
	Minimum Value in this study	0.2	2	2.1	1	1.1	0.6	0.02	0.5
	Threshold (Wilson and Jeffrey, 1987)	1.5	100	100	50	100	50	1.5	7.5
Sediment Quality Guideline-Quotient (SQG-Q)	PEL (Macdonald *et al.*, 1996)	4.21	112	271	108	41.6	160	0.7	-
Metal Pollution Index (MPI)	-	-	-	-	-	-	-	-	-
Index for Ratio-to-reference (I)	Reference stations	0.6	3.09	9.52	3.5	7.41	1.85	0.066	-
Index for new Maximum RTR (NI)	Maximum RTR value	13.3	22.3	53.27	54.57	7.8	34	10.5	-
Marine Sediment Pollution index (MSPI)	Percentile 0-20	0.6	3.3	15.4	3.0	7.0	2.0	0.060	-
	Percentile 20-40	1.0	5.0	34.0	6.0	8.0	5.0	0.070	-
	Percentile 40-60	1.5	8.0	57.0	12.0	10.2	9.2	0.080	-
	Percentile 60-80	2.9	18.2	101.6	30.6	21.0	19.6	0.232	-
	Percentile 80-100	8.0	69.0	507.0	191.0	58.0	63.0	0.7	-

Table 8.3 – Classification of dredge material in coastal zones according to DR (1995).

Classes/contaminants (mg/kg)	Cd	Pb	Zn	Cu	As	Cr	Hg
Class 1 – clean dredged material	<1	<50	<100	<35	<20	<50	<0.5
Class 2 - trace contaminated dredged material	1-3	50-150	100-600	35-150	20-50	50-100	0.5-1.5
Classe 3 – few contaminated dredged material	3-5	150-200	600-1500	150-300	50-100	100-400	1.5-3.0
Class 4 – contaminated dredged material	5-10	500-1000	1500-5000	300-500	100-500	400-1000	3.0-10
Class 5 – highly contaminated dredged material	>10	>1000	>5000	>500	>500	>1000	>10

For PLI calculation the minimum found in all stations was used as baseline values for each contaminant, since in our sampling points some metal concentrations were lower than the Baseline values proposed by Wilson and Jeffrey (1987). The use of Baseline values would then produce an error in the index calculation (Table 8.2).

Probable Effect Level (PEL), classification of toxic effects, was used for SQG-Q Index calculation. Associated with this guideline there is also the Threshold Effect Levels (TEL), below which there is no toxic effects, developed by the same authors (MacDonald *et al.*, 1996). Although the PEL and TEL were originally developed for coastal waters, their use can be applied in Sado estuarine study area with more confidence due to low range of salinity (from 29 to 37 ‰ Rodrigues and Quintino, 1993).

To evaluate the relation between the contaminants concentrations and Indices, Non-parametric Spearman Coefficients were computed. For index performance evaluation the indices were scored from 1 (lowest classification) to 3 (highest classification) according to indicators criteria and general guidelines like:

- Comparability - existence of a target level or threshold against which to compare it so that users are able to assess the significance of the values associated with it;
- Representative - ability to provide a spatial representative picture of estuarine environmental state and impacts;
- Credibility - good theoretical base in technical and scientific terms; application to estuaries;
- Simplicity - ease of calculation and interpretation;
- Sensitivity and robustness - responsiveness to change in the environment;
- Acceptable levels of uncertainty.

In each management unit the indices were calculated using the median values of chemical concentration in all the locations belonging to each management area. The Mode was also used in the case of the index being nominal. These measures of central tendency were used instead of average since average should only be used for Normal distributions and due to outliners (Wheater and Cook, 2002).

Statistical analyses were conducted using Statistica® 6.0 software. To visualize the index results within Coastal area of Sado Estuary and in management units ArcGIS 8.0® GIS software was used. The kriging interpolations of the contaminant concentractions were computed with Geostatistical Analyst® ArcGiS 8.0 extension. The classification of the classes to visualize the indices was defined based on the literature, when available (in the case of DC, SQG-Q, MSPI, see Table 8.1). For I and NI an equal interval was used for values above the reference stations. In case of MPI and PLI a geometric increment was employed. Their classification was done according to earlier knowledge of sampling station contaminants status and according to the other index classification.

8.3 RESULTS AND DISCUSSION

Regression analyses using less-absolute-values function, and Quasi-Newton non-linear estimated method, for each metal concentration are shown in Fig. 8.2.

Metals and metalloids frequency distributions were positively skewed, so log transformation was used for interpolation surfaces of the contaminants (Fig. 8.3) and for further multivariate statistics. For all the contaminants, geometric anisotropy models were fitted visually and spherical models used. All semivariograms display longer ranges in the direction of azimuth 120º, which corresponds to the water flow*.

A PCA was computed with the metals, metalloid, Al, TOC, FF and Eh. The first PCA component analysis explained 79,6 % of the total variance. When only including in the analysis all the contaminants Cd, Pb, Zn, As, Cu, Cr and Hg the first component explained 83.6 % of the variance. This later PCA factor loadings were used for MSPI calculation and the PCA factor scores were used to compare the differences between the references and impact stations (for I and NI indices). The reference stations were different from the other stations (ANOVA, F = 20.36 p=0.000023), and clustered in the same group.

The results of the indices per location and per area are shown in Fig. 8.4. In Table VII.1 in Annex VII are listed the results of the indices and of the physical and chemical parameters in the 78 locations.

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* Cross-validation procedures (see Annex IV) were computed to evaluate the impact of the semivariogram model on interpolation results.

8.3.1 Background enrichment per contaminant

From the outliners shown in all the regressions of Fig. 8.2, a metal enrichment can be confirmed in the stations with high levels of anthropogenic contamination located in the North Channel: station 34, 35 and 68 near the power plant and ferment industries and 43 near Shipyard (Fig. 8.3). For most of the metals these stations shown levels of enrichment what is also in accordance with spatial distribution of the metals and metalloid where “hotspots” are found close to those anthropogenic sources (Fig. 8.3). In the specific case of Lead, other enriched stations are located near the outfall of Setúbal City and fish ports (stations 1, 2, 17, 19) and station 43 and 139 near the shipyard (Fig. 8.1, 8.2 and 8.3). Other works conducted in the study area also related lead with urban contamination (Vale and Sundby, 1980). Also, stations near those ports (1 and 17) and near pulp and paper industry (40) are enriched in Hg. Station 93 is also enriched in As, reaching its higher value in this station (59.0 mg/kg). One of the major sources of Arsenic is pesticides and herbicides (Donze *et al.*, 1990). This station is located in the middle of the estuary between the sandbanks. Its high arsenic level should be related with water currents and a high sediment deposition rate in the area. According to Neves (1985), the residual flow in the outer estuary shows one cyclonic vortices centred at the outer point of the Sandbanks. The station near the Shipyard (43) had the highest values of Pb (69.0 mg/kg), Zn (507.0 mg/kg), Cu (191.0 mg/kg). This area is under the influence of wastewater and water runoff from that industry (rich in heavy metals). The most important uses of Zn are protection against corrosion, Cu is used in construction materials and Pb is used in paints, pigments and glass (Donze *et al.*, 1990). The station near the power plant and ferment industry (34) had the highest value of Cd (8.0 mg/kg) and Cr (63.0 mg/kg). Sources of Chromium are associated with chemical manufacture, chrome plating and cooling towers (McConnell *et al.*, 1996). Anthropogenic sources of Cadmium could be pesticides and pigments. Also in this area (Station 68) the highest values of mercury (0.7 mg/kg) were found. This metal is released into the environment by human activities such as the combustion of fossil fuels, waste disposal and industrial activities (Donze *et al.*, 1990). Associated with this power plant is the discharge of heavy metals, oils, salts, acids and alkalines. Associated with the ferments industry are organic acids and sulphates (Catarino *et al.*, 1987). Earlier works associated Cd and Zn with sediments deposited in the upper limit of the estuary related with river input (Quevauviller *et al.*, 1989) but this area was not covered by our study.

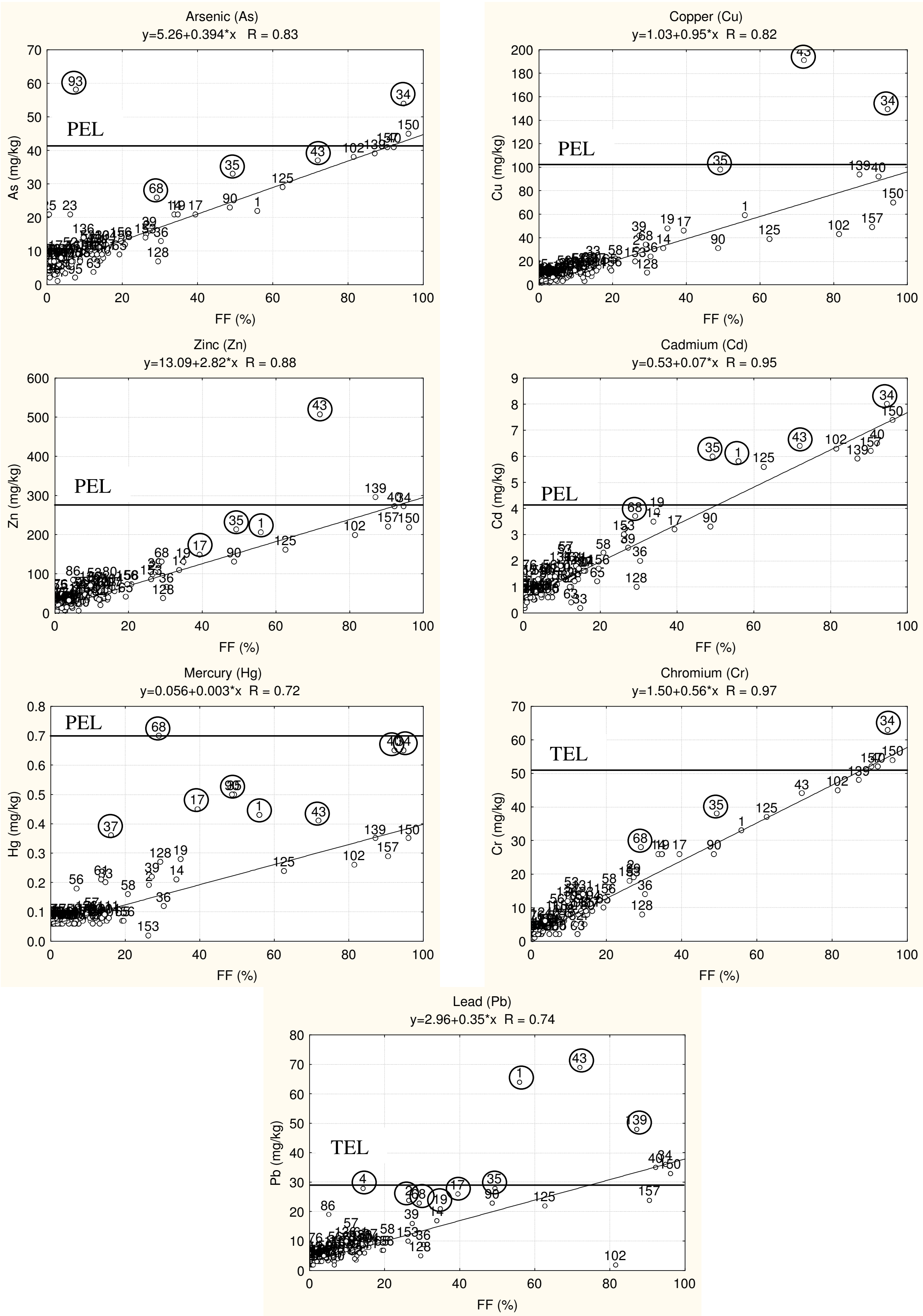

Figure 8.2 – Background enrichment of each heavy metal using robust regression. Lines represent PEL or TEL when concentration values were lower, for each metal. Examples of outliners are shown in circles.

Near the left side entrance of the Alcácer and Águas de Moura Channels (stations 102, 153, 156 and 157 – Fig. 8.1) it can be found an increase in metal's concentration, specially in Cd, Cr, Cu, As and Zn (Fig 8.3). These locations are associated with low hydrodynamics and low depths, so high organic loads can also be associated with non-point pollution runoff and deposition, owing to aquaculture and rice field activities located upstream of those channels.

Alcácer channel can also be a source of heavy metals due to pyrite outcrop erosion and old mining activities in the river drainage basin, as already stressed by other authors (Quevauviller *et al.*, 1989, Cortesão and Vale, 1995).

The concentrations of metals and metalloids are similar to the results presented in other works recently developed in different parts of the outer estuary. In these studies higher contamination was found near the power plant, ferment industry and Eurominas industry. Exception wer only noticed for higher values of Cadmium obtained here when compared to Vale *et al.* (1997) and Gil *et al.* (1999). Also our concentrations are similar to measurements performed 20 years ago in terms of Zn, Cu and Pb (Vale and Sundby, 1980). Dredge operations in superficial sediments and industrial wastewater treatment improvements can explain this stability of contamination levels.

In general metals have similar distribution and are associated with similar urban and industrial point sources as can be seen from Fig. 8.3 and as also confirmed by the PCA. Nevertheless Cd and As showed levels of concern followed by Cu and Zn. The Pb, Cr, and Hg showed only trace contamination (Fig. 8.2 and 8.3).

8.3.2 Contamination by management unit

The different indices showed spatial patterns similar to those of the heavy metals which led to the same management units showing concerning levels (Fig. 8.4). These areas as already indicated above, are located on the North Channel near some industries: one near shipyard and Eurominas; one near pulp and paper industry; one near power plant and ferment industry and one near the outfall of City of Setúbal and fish and urban ports. Also a small unit at the entrance of Águas de Moura channel has higher pollution levels. According to all the indices the large area at the entrance of the estuary, the two areas at the right side entrance of Águas de Moura, and two small areas near the smallest sandbank are unimpacted areas.

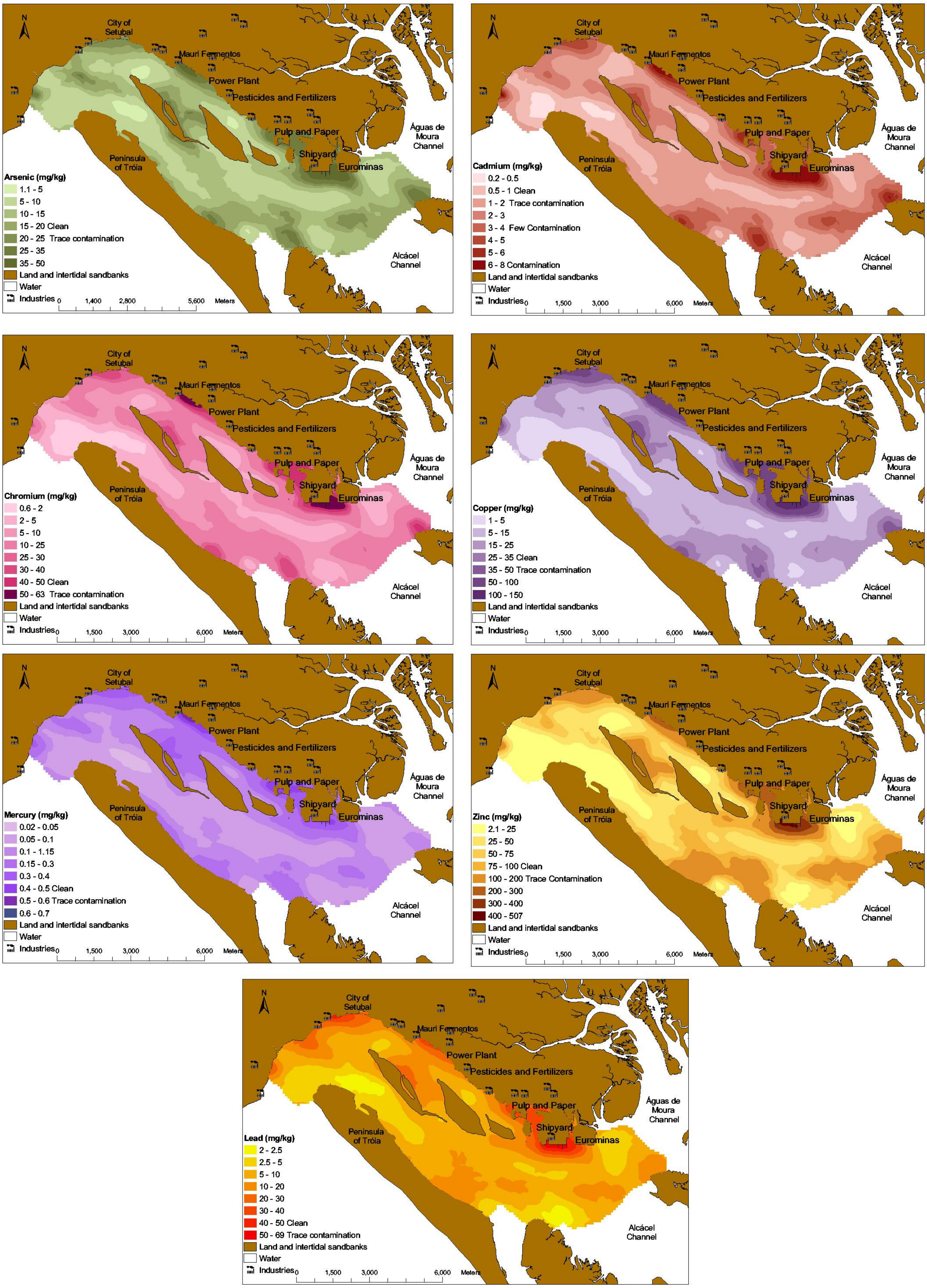

Figure 8.3 – Spatial distribution of the metals in Sado Estuary. Classification according to DR (1995). Industries adapted from Araujo *et al.* (2002).

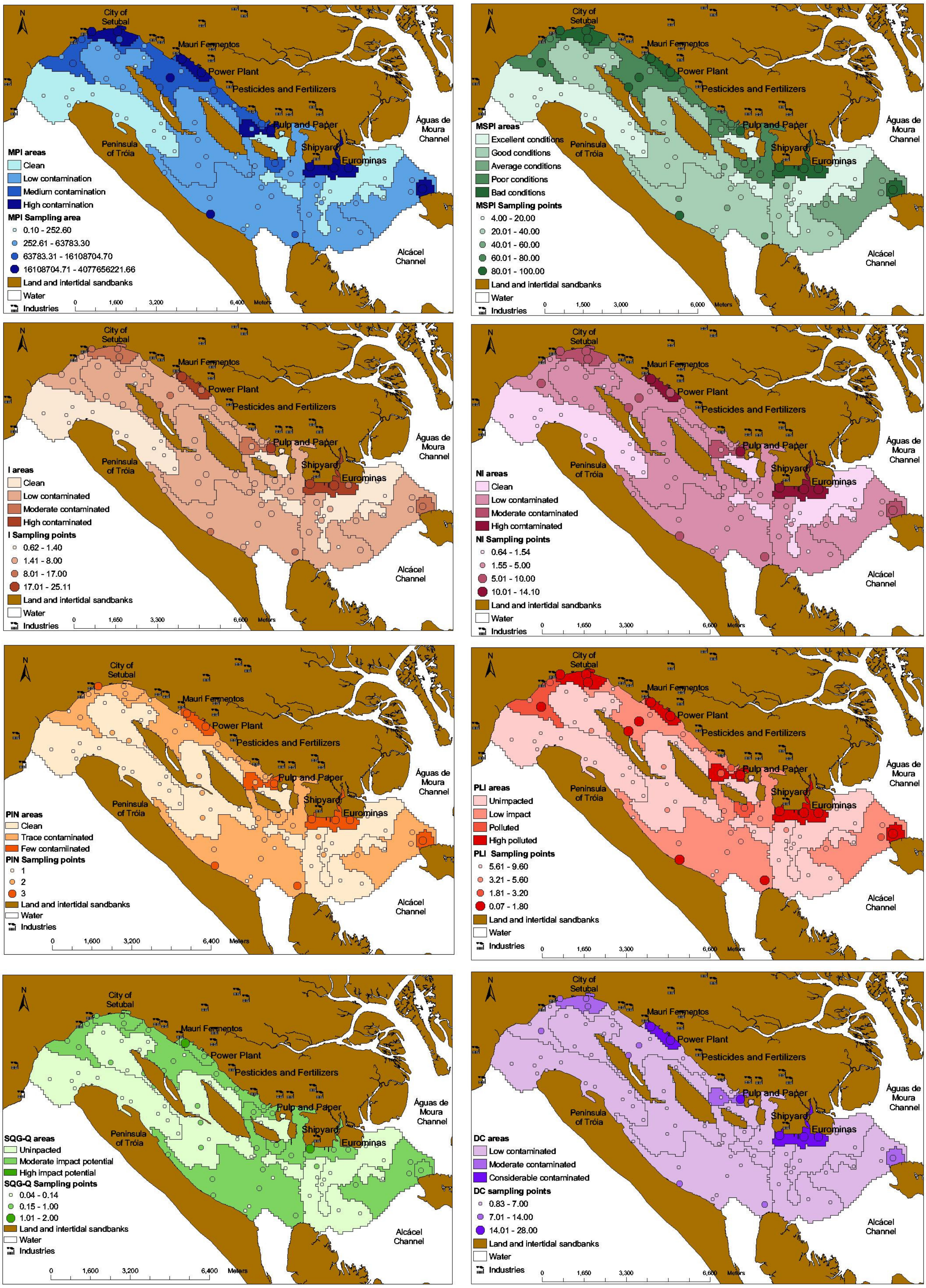

Figure 8.4 – Results of the indices to assess coontamination in the sampling points and management units in the Sado Estuary. Industries adapted from Araujo *et al.* (2002).

8.3.3 Index comparison

All the indices are significantly correlated ($p< 0.05$) between each other and between each contaminant. The similar spatial pattern of contamination and the strong correlation between each contaminant helps this agreement (Table 8.4).

Spatial care must be taken when comparing the different thresholds (Table 8.2) and classification indices (Fig. 8.4). For example since MPI does not compare the contaminants with any guidelines, the classes defined were classified according to earlier knowledge of the sampling station contaminants status and according to the other indices classification. Nevertheless geometric average, as stressed by Ott (1978), has advantages when compared with other aggregations methods (like arithmetic averages used in the other indices except PLI), since it highlights concentration differences.

Although I and NI compare the contaminant concentrations with reference stations, they do not allow to compare the classifications with other ecosystems and their class's definition is also biased. NI compared with I has the advantage to normalize the index values by the more contaminated station (maximum) and to mask outlier values (DelValls *et al.*, 1998b). Even so, their map visualization is equivalent in terms of classification units (Fig. 8.4).

MSPI has a great advantage over the other indices since it gives different weights to each contaminant and it is site-specific. Shin and Lam (2001) suggest that this index could reflect the state of the benthic communities and toxicity level of the sediment. Also the application of a PCA to identify important variables from a monitoring program can reduce sampling resources. Parameters that do not show significant spatial variations can be analysed in a lesser frequency than those that were identified to be more important from the results of the PCA (Shin and Lam, 2001). Given that our stations vary from unpolluted to highly-polluted stations and the stations can be rated from best to worst quality based on dataset percentiles, it allows a more accurate index classification. The problem arises when comparing the results with other ecosystems with different datasets. Also if for a study area in the dataset there aren't high contamination differences the index classification may be biased.

Table 8.4 – Spearman correlation between the indices, contaminants and sediment characteristics. All correlations are significant ($p < 0.05$).

	Cd	Pb	Zn	Cu	As	Cr	Hg	TOM	FF	Eh	Al	PIN	DC	PLI	SQG-Q	MSPI	I	NI	MPI
Cd	**1.00**	0.80	0.89	0.90	0.79	0.92	0.76	0.78	0.83	-0.70	0.86	0.89	0.94	-0.95	0.92	0.93	0.92	0.91	0.94
Pb	0.80	**1.00**	0.86	0.83	0.73	0.83	0.73	0.77	0.80	-0.71	0.82	0.79	0.84	-0.88	0.86	0.89	0.89	0.87	0.89
Zn	0.89	0.86	**1.00**	0.90	0.79	0.92	0.71	0.81	0.88	-0.76	0.89	0.84	0.91	-0.95	0.93	0.93	0.97	0.92	0.95
Cu	0.90	0.83	0.90	**1.00**	0.83	0.94	0.79	0.86	0.90	-0.76	0.91	0.85	0.94	-0.95	0.94	0.96	0.95	0.94	0.95
As	0.79	0.73	0.79	0.83	**1.00**	0.84	0.66	0.72	0.76	-0.59	0.78	0.83	0.91	-0.85	0.91	0.85	0.87	0.91	0.86
Cr	0.92	0.83	0.92	0.94	0.84	**1.00**	0.76	0.88	0.93	-0.78	0.93	0.88	0.95	-0.97	0.95	0.96	0.96	0.95	0.98
Hg	0.76	0.73	0.71	0.79	0.66	0.76	**1.00**	0.68	0.74	-0.66	0.72	0.67	0.77	-0.78	0.77	0.84	0.76	0.77	0.80
TOM	0.78	0.77	0.81	0.86	0.72	0.88	0.68	**1.00**	0.95	-0.76	0.86	0.78	0.82	-0.88	0.84	0.85	0.86	0.85	0.87
FF	0.83	0.80	0.88	0.90	0.76	0.93	0.74	0.95	**1.00**	-0.81	0.92	0.82	0.88	-0.93	0.89	0.90	0.91	0.90	0.92
Eh	-0.70	-0.71	-0.76	-0.76	-0.59	-0.78	-0.66	-0.76	-0.81	**1.00**	-0.78	-0.69	-0.73	0.78	-0.74	-0.77	-0.77	-0.75	-0.77
Al	0.86	0.82	0.89	0.91	0.78	0.93	0.72	0.86	0.92	-0.78	**1.00**	0.83	0.88	-0.92	0.89	0.90	0.91	0.89	0.92
PIN	0.88	0.74	0.82	0.83	0.82	0.85	0.67	0.72	0.77	-0.65	0.80	**1.00**	0.90	-0.87	0.88	0.85	0.86	0.88	0.88
DC	0.94	0.84	0.91	0.94	0.91	0.95	0.77	0.82	0.88	-0.73	0.88	0.91	**1.00**	-0.97	1.00	0.96	0.97	0.99	0.98
PLI	-0.95	-0.88	-0.95	-0.95	-0.85	-0.97	-0.78	-0.88	-0.93	0.78	-0.92	-0.91	-0.97	**1.00**	-0.98	-0.97	-0.99	-0.97	-0.99
SQG-Q	0.92	0.86	0.93	0.94	0.91	0.95	0.77	0.84	0.89	-0.74	0.89	0.90	1.00	-0.98	**1.00**	0.96	0.98	1.00	0.98
MSPI	0.93	0.89	0.93	0.96	0.85	0.96	0.84	0.85	0.90	-0.77	0.90	0.88	0.96	-0.97	0.96	**1.00**	0.97	0.96	0.98
I	0.92	0.89	0.97	0.95	0.87	0.96	0.76	0.86	0.91	-0.77	0.91	0.89	0.97	-0.99	0.98	0.97	**1.00**	0.99	0.99
NI	0.91	0.87	0.92	0.94	0.91	0.95	0.77	0.85	0.90	-0.75	0.89	0.89	0.99	-0.97	1.00	0.96	0.99	**1.00**	0.98
MPI	0.94	0.89	0.95	0.95	0.86	0.98	0.80	0.87	0.92	-0.77	0.92	0.90	0.98	-0.99	0.98	0.98	0.99	0.98	**1.00**

The PIN index has the advantage of being simple to compute and to give the results according to dredged material classes of the Portuguese law. This allows the comparison with other ecosystems. The problem is the low sensitivity to toxicity effects of the thresholds of the sediment defined in the law classification. Using PIN index our stations are only classified up to the level 3 of “few contaminated”, when in the other indices high pollution levels are found (for example as shown in Fig. 8.4, stations 34 and 43 are considered with high impact potential for adverse biological effects according to SQG-Q index but according to PIN they have only low contamination). This is due to PEL thresholds (concentration above which adverse effects frequently occur) being considered only as trace contamination (Class 2) by the Portuguese law (see Table 8.2 and 8.3).

PLI also allows the comparison of the results with other ecosystems. For example the worst polluted station has a PLI value of 0.07 (station 43). This value is low when compared with other European highly contaminated estuaries like Tolka or Avoca in Ireland where PLI values of 4.3×10^{-3} and 10^{-6} were obtained (Wilson and Elkaim, 1991). For the calculation of this index the Threshold and Baseline values (see Table 8.1) were determined specifically for estuaries in which these values have been found for sediment contamination in conjunction with depleted biological communities. The problem is that they were never updated after their first publishing (Jeffrey *et al.,* 1985 *fide* Wilson and Elkaim, 1991). Also the Baseline values defined by the authors are higher than those found in our reference stations which resulted in erroneous PLI calculations and made it necessary to use our baseline values. Nonetheless, the sandy granulometry of our reference stations sediments can explain these lower values.

SQG-Q also allows the comparison with other ecosystems, the guidelines used are recent and their predictive ability was largely tested (e.g. Macdonald *et al.*, 1996, DelValls and Chapman, 1998, Long *et al.*, 1998, Long and MacDonald, 1998, Hyland *et al.*, 1999, Long *et al.*, 2000). However, no maximum level is established and the SQG are not site-specific. Hyland *et al.* (1999), found degraded benthic assemblages with mean SQG-Q < 0.1, i.e. with a much lower range in concentrations of sediment contaminants. Regional variations in the magnitude of sediment contamination, the insensitive indicators of toxicity used by Long *et al.* (1998), the measure of benthic community conditions that reflex the sensitivities of multiple component species to longer-term exposures and potential interactions may explain some of the differences that were observed in adverse bioeffect levels. Although the use of empirically derived SQG in sediment monitoring and assessment has been subject to debate, recent studies suggest that SQG continues to be widely used to predict when chemical concentrations are likely to be associated with a measurable biological response (Fairey *et al.,* 2001).

The DC index classifies most of the estuary management units with low impact. Although already tested successfully in coastal areas, the use of background levels defined for lakes may have induced underestimation. Also the problem concerning natural background levels has already been well discussed and can vary from general geological reference levels to a pre-industrial or pre-civilization level for every location (Kwon and Lee, 1998). However, for the calculation of this index it is not necessary reference stations data, like in I and NI. This data is not always available for each ecosystem.

The indices were scored according to indicators criteria and general guidelines and considering the above indices discussion (Table 8.5). In an overall comparison the index SQG-Q has the highest score and MPI has the lowest.

Table 8.5 – Score of the metal assessment indices, based on several criteria.

	PIn	DC	PLI	SQG-Q	I	NI	MSPI	MPI
Simplicity	3	3	3	3	3	3	2	3
Representative	3	3	3	3	2	2	3	1
Credibility	3	1	2	3	3	3	3	2
Comparability	3	3	3	3	1	2	2	1
Sensitivity and robustness	2	3	3	2	3	3	3	1
Acceptable levels of uncertainty	2	2	2	3	2	2	3	2
Total	16	15	16	17	14	15	16	10

The metal assessment indices have different aims, since some evaluate the potential toxicity for adverse biological effects, while others just measure a contamination enrichment levels. Due to these differences comparation should be made with special caution.

The use of the multiple indices or approaches available are recommended for a better assessment of the quality of sediments and its evolution and they are relatively simple to apply and rapid (Kwon and Lee, 1998). The use of these kind of tools give confidence in making decisions about and ecosystem and human heath protection using.

Most of these indices, with the exception of MSPI, gave the same weighs to contaminants mixture or not account for synergies between contaminants like what exists in nature. Weighting is possible but of questionable value. For example, it does not appear reasonable to weight certain chemical contaminants as more important than others, although a criterion could be whether or not they cause any type of adverse effect (Chapman, 1996). The use of PCA in the MSPI index allows the successful assessment of the source of contamination, since this multivariate analysis tool does not need any linear assumption and establishes and quantifies the correlations among the original variables in the data set when the goal is to reduce the number of variables (DelValls *et al.*, 1998a).

8.4 CONCLUSIONS

The tools - interpolation surfaces, GIS and Indices - used in this work for evaluation of sediment estuarine contamination showed to be very useful for aggregation, data transmission and visualization. The use of data aggregation in indices and their visualization using GIS, including the full GIS capabilities, like for example allowing versatility in making spatial queries, has many advantages. These tools are essential for decision making processes and management of natural resources. Loss of information can occur during the conversion of multivariate data into single indices, however, such indices offer useful information, provided that their limitations are recognized.

Different metal assessment indices were used and discussed. Some indices give equivalent information but others give complementary information that can be developed for different purposes. There should be better methods of standardization for Indices to allow better comparability between each other (since several assess the same information).

From the indices used and evaluated SQG-Q had the highest score according to the indicators criteria used but this index of ecological risk assessment can be complemented with the contamination MSPI index. MSPI doesn't normalize the concentrations by ecological risk guidelines and the results from one site are more difficult to compare with other ecosystems, but it allows a more site-specific and accurate information.

In general the Sado estuary has a low contamination level and a moderate potential for observing adverse biological effects. From all the stations analysed, only 3 % are highly contaminated and with high potential for observing adverse biological effects, but 47 % have moderate potential for observing adverse biological effects. Nevertheless some hot spots were found near industrialized zones and in sediments rich in organic matter areas, at the entrance of channels. All metals have similar spatial behavior and are mainly related with deposition areas. Metals of concern are Cd and As followed by Cu and Zn; Pb, Cr, and Hg have shown only trace contamination. In the near future a new urban and industrial wastewater treatment plant will start working so a water quality improvement will be expected.

To better link and evaluate the indices results with the pressures on the estuary, like urban and industrial wastewater discharges and water runoff, a sediment transport model should be used to estimate which estuary management unit will suffer an effect caused by a pressure and the resulting impact (Painho *et al.*, 2002 – see Annex II).

Heavy metals assessment indices should not be used as the sole line of evidence of sediment quality. In future developments organic compounds (pesticides, PAHs and PCBs) will be integrated in the contamination evaluation, which can be correlated with different data pollution sources and spatial distribution. Furthermore the integration of the contamination with biota and toxicity evaluation will be conducted in each management unit for a weigh of evidence to assess the sediment quality.

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CHAPTER 9 – BENTHIC BIOTOPE INDEX DEVELOPMENT FOR THE SADO ESTUARY: PORTUGAL

BENTHIC BIOTOPE INDEX DEVELOPMENT FOR THE SADO ESTUARY: PORTUGAL

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ABSTRACT

An integration of sediment physical, chemical, biological, and toxicity data is necessary for a meaningful interpretation of the complex sediment conditions in the marine environment. Benthic community's assessment is one of the vital components for that interpretation, yet their evaluation is complex and requires large amounts of time and money. Thus, there is a need for new tools that are less expensive and more understandable for managers. This paper presents a benthic biotope index to predict the occurrence of macrobenthic communities, from physical and chemical variables. Parameters like sediment type, organic matter, depth and hydrodynamic parameters were selected, through a discriminant analysis, to compute the index. The benthic biotopes used were previously delineated for the Sado Estuary by other authors based on multivariate methods. The index demonstrated to be a valid tool to assess the spatial patterns of benthic habitat and to synthesize stress biotope gradients.

KEYWORD: Benthos, index, estuaries, pollution effects, sediment quality assessment, biotope gradients

9.1 INTRODUCTION

The study of benthic communities is one of the crucial components to monitor the environmental health of estuaries. Macrobenthic fauna provides an ideal measure of the biota's response to environmental disturbance and are an effective indicator of the extent and magnitude of pollution impacts in estuarine environments (Warwick and Clarke, 1993, Engle *et al.,* 1994, Weisberg *et al.*, 1997, Borja *et al.,* 2000). Their advantages as pollution indicators are the followings: i) they are direct measures of the condition of the biota and may uncover problems undetected or underestimated by other methods (Borja *et al.,* 2000); ii) their limited mobility prevents them from escaping adverse conditions like hypoxia accumulation of anthropogenic contaminants (Ranasinghe *et al.,* 1994, Weisberg *et al.,* 1997, Paul *et al.,* 2001); iii) they integrate responses to exposure and respond to multiple stressors over relatively long periods of time (Ranasinghe *et al.,* 1994, Ranasinghe *et al.,* 2002); iv) they have a taxonomic diversity that can usually be classified into different functional response groups (Smith *et al.,* 2001).

Benthic communities are often associated with natural habitat gradients such as salinity and sediment type (Manninom and Montagna, 1997, Engle and Summers, 1998, Paul *et al.,* 2001). Grain size data may be used to determine the extent of recovery from sedimentary disturbance, to evaluate the benthic habitats and the structure of benthic assemblages (Gibson *et al.,* 2000), and to assist in providing early warning of potential impacts to the estuarine ecosystem (Gibson *et al*., 2000). The silt-clay content of sediments (the fraction <63 µm) is an important factor determining the composition of the biological community at a site, and is therefore important in the assessment of the benthic community (Strobel *et al*., 1995). Benthic habitat gradients can also be distributed according to depth (Clarke, 1993). The fact that shallow assemblages are defined by a combination of depth and sediment type is consistent with the theory that the hydrodynamics energy profile at the bottom is the controlling factor (Gibson *et al*., 2000). The energy profile of water flow immediately above the sediment-water interface determines the size of particles in superficial sediment, which in turn affects benthic properties. Depth affects the energy profile because the effects of wave energy on the bottom are usually greatest in shallow areas and decrease as the distance between the surface and bottom increases (Bergen *et al*., 2001). Hydrodynamic events can also have a strong effect on hypoxia variation in frequency and severity. Hypoxia and organic enrichment bring significant structural changes in benthic communities and energy flow processes (Pearson and Rosenberg, 1978, Diaz and Rosenberg, 1995, Diaz, 2001).

Characteristics of benthic assemblages expressed as indices have been used to measure ecological status and trends of marine and estuarine environments for several decades. An index based upon several structural properties of benthic environment and/or sediment type, can summarize the benthic data and characterize estuarine biological condition.

Benthic indices generally fall into three types of increasing complexity and information: i) *single community* attribute measures or individual-species data combination, including species diversity or abundance/biomass ratios, are used to summarize data beyond the level of individual species; ii) *multi-metric* index approach are used to combine multiple measures of community response into a single index to more effectively capture the different types of response that occur at different levels of stress; iii) *multivariate methods* species composition information is used by describing the assemblages pattern in a comparative multivariate space, based upon a pollution tolerance is scored (Smith *et al.*, 2001). A fourth type can also be considered when the index is calculated based only on the *sediment habitat* type, using a combination of physical and chemical data.

The use of single indicators has not proven to be ideal for monitoring estuarine environments, which experience highly variable natural conditions (Engle *et al.,* 1994). Multivariate approaches can provide higher sensitivity in characterizing benthic patterns (Warwick and Clarke, 1991, Clarke, 1993) but their assessment and output are usually too complex to present in a easy and understandable way to managers (Clarke, 1993, Smith *et al.,* 2001). On the contrary, indices allow one to integrate and simplify a mass of heterogeneous data, leading to better communication between scientists and non-specialists and easier interpretation whereby quality and management goals can be set (Wilson and Jeffrey, 1994, Alden *et al.*, 2002). These qualities compensate for any sacrifice of scientific data (Wilson and Jeffrey, 1994).

Table 9.1 presents a chronological list of benthic indices applied to estuarine ecosystems including data source and classification type. Only a few of the diversity indices are listed. Their uncritical use, as a unique index, in estuarine situations has been deemed inappropriate. This is due to low number of species that are naturally found in estuaries and the response of this index, which to any environmental stress mimics the response to pollution (Wilson and Jeffrey, 1994).

The indices listed in Table 9.1 are applicable across habitat boundaries and have been developed for estuaries and coastal areas in several geographic sites around the world. Most of these indices are intended to identify degraded benthic invertebrate assemblages that are indicative of low dissolved oxygen concentrations in bottom water or high concentrations of chemical contaminants in sediment which have common pollution effects in estuaries (Ranasinghe *et al.*, 2002). Some of the most recent indices have been rigorously verified through multivariate statistical analyses (Rakocinski *et al.*, 1997, Alden *et al.*, 2002) and compared between each others (Ranasinghe *et al.*, 2002). Most of these indices require large benthic metrics databases and need a previous classification of uncontaminated reference stations (e.g. Engle and Summers, 1999, Paul *et al.*, 2001, Alden *et al.*, 2002), which sometimes are difficult to locate and vary for unknown reasons often unrelated to contamination (Anderson *et al.,* 1998).

Table 9.1 – Literature review of macrozoobenthics indices applied to estuarine ecosystems.

Author	Year	Index name	Data source	Type of index
Gleason (1922)	1922	• Gleason Diversity Index (G)	Benthic metrics	Single community
Shannon and Weaver (1949)	1949	• Shannon-Wiener Diversity Index (H)	Benthic metrics	Single community
Leppakowski (1975)	1975	• Benthic Pollution Index (BPI)	Benthic metrics	Single community
Word (1978, 1979) *fide* Bascom (1982)	1978	• Infauna Trophic Index (ITI)	Benthic metrics	Multi-metric
Bellan (1980); Bellan *et al.* (1988)	1980	• Annelid Index of Pollution (AIP)	Benthic metrics	Single community
Satsmadjis (1982) *fide* Satsmadjis (1985)	1982	• Pollution Coefficient (P)	Benthic metrics and physical parameters	Multi-metric
Jeffrey *et al.* (1985)	1985	• Biological Quality Index (BQI)	Benthic metrics	Multi-metric
Rhoads and Germano (1986) Diaz *et al.* (2003)	1986	• Organism-sediment index (OSI)	Sediment profile images	Sediment habitat
Chapman *et al.* (1987)	1987	• Summary index for benthic infauna Ratio-to-Reference of Sediment Quality Triad (RTR)	Benthic metrics	Multi-metric
Majeed (1987) Grall and Glémarec (1997)	1987	• Biotic Indices (BI)	Benthic metrics	Multi-metric
McManus and Pauly (1990)	1990	• Shannon-Weiner evenness proportion Index (SEP)	Benthic metrics	Single community
Weisberg *et al.* (1993), Schimmel *et al.* (1994), Strobel *et al.* (1995) Paul *et al.* (1999), Paul *et al.* (2001)	1993	• Benthic index of estuarine conditions (BIEC)	Benthic metrics	Multi-metric
Engle *et al.* (1994) Engle and Summers (1999)	1994	• Benthic condition Index (BCI)	Benthic metrics	Multi-metric
Ranasinghe *et al.* (1994), Weisberg *et al.* (1997), Van Dolah *et al.* (1999), Alden *et al.* (2002)	1994	• Benthic Index of biotic integrity (B-IBI).	Benthic metrics	Multi-metric
Warwick and Clarke (1995)	1995	• Taxonomic diversity index (Δ) • Taxonomic distinctness (Δ*)	Benthic metrics	Single community
Fairey *et al.* (1996) *fide* Anderson *et al.* (1998)	1996	• Relative benthic index (RBI)	Benthic metrics	Multi-metric
Nilsson and Rosenberg (1997)	1997	• Benthic habitat quality Index (BHQ)	Sediment profile images	Sediment habitat
DelValls *et al.* (1998)	1998	• Summary index for benthic infauna new Maximum Ratio-to-Reference of Sediment Quality Triad (RTM)	Benthic metrics	Multi-metric
Roberts *et al.* (1998)	1998	• Macrofauna Monitoring Index	Benthic metrics	Multi-metric
Borja *et al.* (2000), Borja *et al.* (2003)	2000	• Marine Biotic Index (BI)	Benthic metrics	Multi-metric
Ferreira (2000)	2000	• EQUATION index – Sediment quality	Benthic metrics, pollutants, bioacumulation	Multi-metric
Eaton (2001)	2001	• Biocrioteria for estuarine shallow water	Benthic metrics	Multi-metric
Smith *et al.* (2001)	2001	• Benthic Response Index (BRI)	Benthic metrics	Multivariate methods
Degraer *et al.* (2002)	2002	• HABITAT model	Physical and chemical parameters	Sediment habitat
Schmidt *et al.* (2002)	2002	• Modified Ecotoxicological Rating (METR)	Physical, chemical and toxicological parameters	Sediment habitat and Single community

Since the collection of data to retrieve a detailed bathymetric-sedimentological map of an area is less time-consuming than the collection of those for a detailed macrobenthic map, models that provide a powerful time-cost-efficient tool to retrieve a full-coverage view on the spatial distribution of the macrobenthic potential should be used (Degraer *et al.,* 2002). The Indices

OSI, BHQ and HABITAT (Table 9.1) are good examples of how the benthic habitat quality can be assessed using only sedimentological data. METR index add to the sedimentological data toxicity data. These kinds of indices, although being promising to assess benthic system's viability or health (Diaz *et al*., 2003), are still underexplored.

The aim of this work is to develop an index of benthic biotopes, based on physical and chemical variables strongly related with them. Other author previously analyzed the benthic data. The index was developed using a discriminant analysis and applied to Sado Estuary to predict benthic biotopes at new locations where physical and chemical variables were recently measured. This Benthic index will be integrated with contaminants and toxicity indices for sediment quality assessment and represented in management units to be part of a management and data system for Sado Estuary. The management units were delineated based on sediment parameters like Fine Fraction contents (FF), Total Organic Mater (TOM) and redox potential (Caeiro *et al.,* 2003a – Chapter 4).

9.2 METHODS

9.2.1 Study area

The Sado Estuary is the second largest in Portugal with an area of approximately 24,000 ha. It is located in the West Coast of Portugal. Most of the estuary is classified as a Natural Reserve but also with many industries and harbour associated activities mainly on the northern margin of the estuary (Caeiro *et al.* 2002). The Sado Estuary is characterized by a North Channel with weaker residual currents flow and shear stress, that enhance accumulation of sediment allowing locally introduced pollutants settle out rather than be transported away. The southern channel, separated by the North Channel by sandbanks, is highly dynamic and tides are the main responsible for the water circulation. Geometric characteristics distinguish the outer estuary (our study area) from the inner estuary, corresponding to a narrow channel (Alcácer channel). The inner part of the outer estuary, (entrances of Águas de Moura and Alcácer Channels), is quite shallow with tidal flats (Rodrigues and Quintino, 2002)

9.2.2 Benthic biotopes of Sado Estuary

A benthic survey was undertaken in the outer estuary in 1986, where superficial sediments and macrofauna were sampled at 131 locations (Rodrigues, 1992). This study allowed the classification of benthic biotopes obtained through classification analysis (TWINSPAN cluster classification). To evaluate the relation between those biotopes and the prevailing hydrophysical and sedimentary conditions in the outer estuary, ordination analyses (canonical correspondence and simple correspondence) were performed on the following physical and chemical parameters: Fine Fraction (FF), Sand, Gravel, Total Organic Matter (TOM), Depth, Shear Stress, Velocity, Temperature and Flow. The ordination analyses suggested a very good agreement between the conclusions drawn from the analysis of the biological data alone and those from the imposed variability of the measured physical and chemical variables (Rodrigues, 1992) (Table 9.2 and Fig. 9.1).

Table 9.2 – Summary statistics of the physical and chemical variables in each community type for Sado Estuary (data from Rodrigues, 1992).

	FF (%)	Sand (%)	Gravel (%)	TOM (%)	Shear Stress (Nm^{-2})	Flow (m^2s^{-1})	Velocity (ms^{-1})	Depth (m)
				A_1 *Marine Type*				
Mean	2.1	89.8	8.0	0.5	45.0	7.9	0.4	13.4
Standard deviation	1.5	11.5	10.5	0.1	16.7	5.2	0.2	9.1
				A_2 *Marine impoverished*				
Mean	13.9	85.7	0.4	2.4	22.6	2.7	0.3	5.9
Standard deviation	33.2	33.0	0.5	4.7	14.5	2.7	0.1	5.2
				B_1 *Transition region*				
Mean	15.8	80.0	4.2	2.2	23.1	3.3	0.3	10.9
Standard deviation	15.4	16.3	7.8	1.6	13.1	2.7	0.1	9.0
				B_{2a} *Estuarine type*				
Mean	24.7	73.5	1.9	2.5	27.7	2.5	0.3	6.6
Standard deviation	18.0	17.2	2.6	1.9	11.7	1.5	0.1	3.4
				I *Estuarine enrichment*				
Mean	41.2	57.4	1.4	5.1	15.4	1.9	0.2	6.3
Standard deviation	17.1	16.0	3.5	2.1	6.9	1.0	0.1	3.3
				II *Estuarine impoverished*				
Mean	72.6	27.1	0.4	7.6	11.1	1.2	0.2	5.7
Standard deviation	22.0	21.2	0.8	3.4	8.5	0.8	0.1	2.1
				B_{2b} *Estuarine highly disturbed*				
Mean	75.1	23.6	1.3	9.8	4.6	0.4	0.1	4.3
Standard deviation	27.9	25.6	2.5	2.3	6.8	0.6	0.1	0.6

The benthic biotopes assessed in (Rodrigues, 1992) study were (Table 9.2 and Fig. 9.1):

Marine type (A_1) -13 stations- This community corresponds to the clean coarse sands of the mouth of the estuary and southern channel with high hydrodynamics and depth. This community was characterized by: mean species richness in each site (*s*) equal to 32 sp per 0.1

m^2, mean biomass per site (*b*) equal to 5.7 g per 0.1 m^2, mean abundance per site (*a*) equal to 218 ind per 0.1 m^2 and species diversity (*H'*) equal to 5.2.

Marine impoverished (A_2) -8 stations- This community is located in the upper region of the estuary, spread over 6 small areas. This community has lower values of *s* (17 sp per 0.1 m^2), *b* (3.1 g per 0.1 m^2), *a* (133 ind per 0.1 m^2) and *H'* (3.2). When compared with the *marine type* community these stations have an increase in silt and total organic matter and the most characteristics species disappear.

Transition region (B_1) -31 stations- This community is located in a large area inside the estuary after the entrance, more through the southern than the northern channel. It is characterized by species of both the *marine* and the *estuarine type* communities, together with an important proportion of species only present in this region. This community showed the highest mean species richness (64 sp per 0.1 m^2) and *H'* (5.8), one of the highest *b* (36.5 g per 0.1 m^2) and *a* (897 ind per 0.1 m^2), and the lowest proportion of species sampled only once in each affinity group, compared with the whole estuary. The mean silt and total organic matter content of the stations belonging to this community type shows an increase, and has a decrease in velocity and flow when compared with the *marine type* community.

Estuarine type (B_{2a}) -43 stations- This community type comprise the majority of the southern channel and the upper part of the estuary. The mean *s* (34 sp. per 0.1 m^2), *a* (402 ind per 0.1 m^2), *b* (17.7 g per 0.1 m^2) and *H'* (4.3) were all lower than observed in the *transition region*, but most of them higher than the ones obtained in the *marine type* community.

Estuarine enriched (I) -19 location- This community is located in the northern channel, mainly in a large area which bordered the northern margin of the intertidal sandbanks. The mean silt, sand, gravel and total organic matter content of this region clearly indicates an increasing fine, organic content, and a decrease in flow, velocity and shear stress in comparison to the estuarine type area. This region showed higher values of *s* (49 sp per 0.1 m^2), *a* (728 ind per 0.1 m^2), *b* (36.8 g per 0.1 m^2) and *H'* (4.7), also compared with *estuarine type,* and the highest proportion of species with sampling frequency higher than 50 %.

Estuarine impoverished (II) -13 stations- This community is located close to the northern margin, in the vicinity of the industrial complex and of the urban sewage outfall, spread over 5 stretch areas. This region is characterized by a clear organic and silt enrichment and a low hydrodynamics and depth as compared to the previously described regions. The stations that comprise this region showed the lowest *a* (105 ind. per 0.1 m^2) and *b* (6.4 g per 0.1 m^2) within the estuarine community. The *s* found in this community type was 18 sp per 0.1 m^2 and the *H'* is 4.6.

Estuarine highly disturbed (B_{2b}) -4 stations- This community comprised the most disturbed areas of the estuarine community. Theses stations are mainly located in 3 small areas in the proximity of the Setúbal city sewage outfall and pulp mill outfall. This community showed the lowest mean species richness (12 sp per 0.1 m^2) and diversity (0.3) of the whole estuary, while the highest means abundance per site (4002 ind per 0.1 m^2). It has a mean biomass equal to 19.6 g per 0.1 m^2. The mean silt, sand, gravel and total organic content of these areas indicate a strong organic enrichment, followed by the lowest hydrodynamics and depth.

Other more recent studies conducted in the estuary showed that overall, biological succession had suffered no significant changes, especially as far as the most characteristics species are concerned. However, recent dredged operations (1995), caused water circulation changes and decreases in the mean content of the fine fraction and organic matter in the sediment at the transition assemblages (Carvalho *et al.,* 2001, Rodrigues and Quintino, 2002).

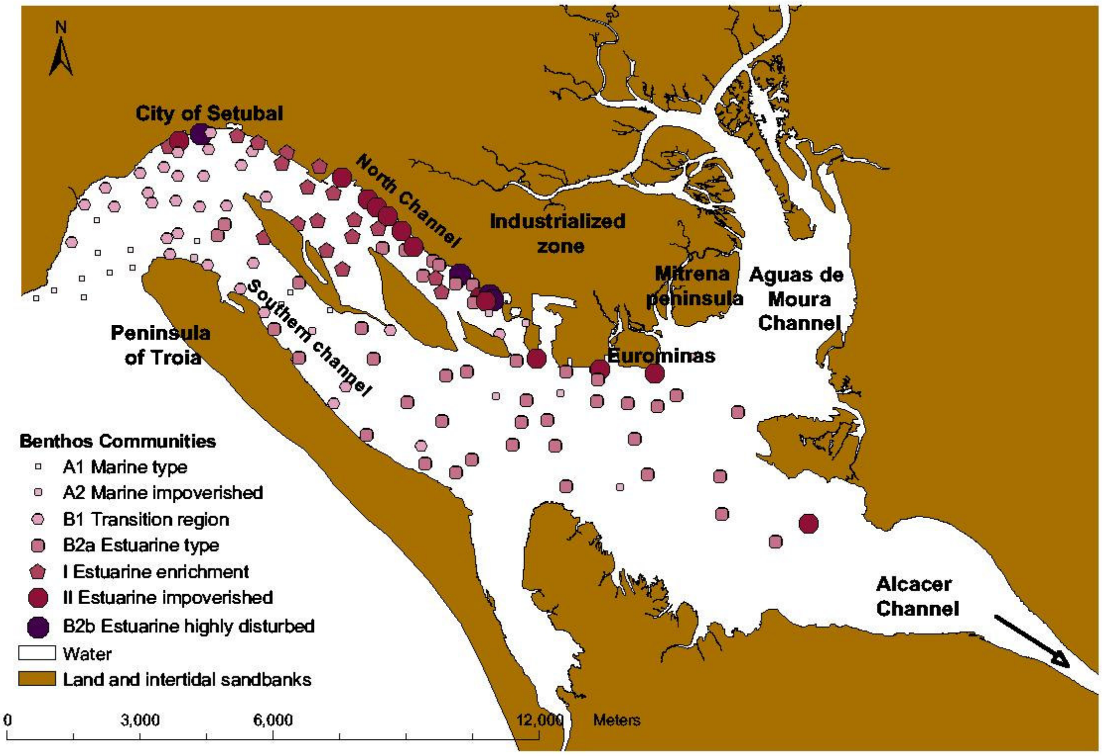

Figure 9.1 – Location map of 131 sampling locations and benthic communities in Sado Estuary. Data from Rodrigues, (1992). Coastal line from Caeiro *et al.,* (2003b).

9.2.3 Index development

Owing to the strong relation found between the benthic communities and the physical and chemical parameters described above, a forward Stepwise Regression Discriminant Analyses (SDA) was applied to the 131 standardized dataset. Discriminant Analysis approach has been largely used to combine benthic metrics into a benthic index (Engle *et al.*, 1994, Strobel *et al.,* 1995, Chaillou *et al.*, 1996, Engle and Summers 1999, Paul *et al.*, 2001) although much less used to combine physical and chemical parameters. This analysis was conducted in order to select a subset of the candidate physical and chemical parameters that best discriminate between the seven benthic biotopes and to determine which linear combination of these variables showed the most substantial difference between those biotopes.

The SDA was computed for *n* variables with *n* steps, F value larger than 1 for variable to enter in the analysis, and a Tolerance value (variable's redundancy) for each variable higher than 0.01.

Temperature parameter was not used in the SDA since it was the weakest environmental factor found in the ordination analysis and it exhibits low variability among communities type. In general the other parameters have averaged values that differ between communities and display a clear gradient from *marine type* to *estuarine high disturbed* communities (Table 9.2). Pearson correlations were calculated for the dataset to determine the presence of any redundancy among variables (Engle and Summers, 1999). The variables were standardized (centred and scaled) to be treated with equal importance.

There was no need to adjust for the effect of salinity, that could reduce the effectiveness of the index (Engle *et al.*, 1994, Paul *et al.*, 2001), since the salinity ranged only from 29 to 37 ‰ in the study area (Rodrigues, 1992).

In order to validate the discriminant function using a jackknife approach, the total data set was divided into a prediction (70% of data) and a validation sub-set according to a proportionately stratified sampling procedure (Hair *et al.*, 1992, Llansó *et al.* 2002, Weigel, 2003). Other proportions for the two subsets were tried to investigate the impact of sampling density on the results.

In order for the predictive accuracy of the discriminant function to be acceptable, it must exceed the percentage of validation data that could be classified correctly by chance. This percentage is calculated using the proportional chance criterion (Hair *et al.,* 1992) as:

$$C_{pro} = \sum_{i=1}^{z} P_i^2 \qquad \text{(eq. 9.1)}$$

where:

C_{pro}= proportional chance criterion

i – index for the z communities (1 to z)

P_i – proportion of individuals in community i.

The maximum chance criterion (C_{max}) was also computed from the percentage of the total sample represented by the largest community group (Hair *et al.,* 1992).

New observation are allocated to the community with the highest standardized total discriminant score from the SDA classification functions with a posterior probability of the predictive choice:

$$S_z = \left(\sum_{j=1}^{n} W_{zj} * V_j \right) + C_z \qquad \text{(eq. 9.2)}$$

where:

S_z –classification score for community z

V_j –observed value for the variable j (1 to n)

W_{zj} – weight for the variable j in community z.

C_z - constant for the community z.

The benthic biotope index (BI_{bio}) values were then calculated to range from 1 to z on a continuous scale, based on the posterior probabilities of occurrence for each observation:

$$BI_{bio} = \sum_{j=1}^{z} Z_i * prob_i \qquad \text{(eq. 9.3)}$$

where:

$Prob_i$– posterior probabilities of occurrence of the corresponding community i

Z_i – Number of the community i, from 1 to z.

The prior classification probability of occurrence is proportional to group size. The communities were numbered from 1 to *z* in accordance to an increase gradient of organic load (from *marine type* to *estuarine high disturbed* communities) according to Pearson and Rosenberg (1978) paradigm.

The BI_{bio} index was used for prediction of the benthic biotopes at 77 stations sampled in the outer Sado Estuary between October of 2000 and January of 2001, where physical and chemical parameters were measured. The 77 sampling design was chosen to assess the sediment quality of management units previously delineated (Caeiro *et al.,* 2004 – Chapter 7). Total Organic Matter (loss on ignition), Fine Fraction (< 63 µm) (hydraulic separation), (Caeiro *et al.*, 2003a – Chapter 4), Sand (63 - 2000 µm) and Gravel (> 2000 µm) (dry sieving) were determined for each location. The values of the hydrodynamic variables for these same locations were predicted using an updated hydrodynamic model previously elaborated for the outer estuary (Martins *et al.,* 2001). Rodrigues (1992) used the same model, for calculation of their hydrodynamic data. The value of the hydrodynamic variables was derived as integration of the transient model results computed over a simulated fortnight time period (330 h) using a time step of 5 min. *Depth*, *water flow* and *velocity* values were calculated using the arithmetic mean of all the instantaneous values for that site during the simulated running period. The maximum value of the simulated running time period was considered for *shear stress* variable at each location.

Statistical analyses were conducted using Statistica® 6.0 software. To visualize the index results within Coastal area of Sado Estuary and management units ArcGIS 8.0® GIS software was used. Geostatistical Analyst® ArcGiS extension was used to perform kriging interpolations of the results. The median values of the stations were calculated for BI_{bio} index visualization in each management unit.

9.3 RESULTS AND DISCUSSION

9.3.1 Index calculation and validation

In the first stepwise discriminant analysis (Model I) Sand and Gravel variables were not included in the model (see Table 9.3). Sand percentages are strongly correlated with Fine Fraction (-0.98, Table 9.4), the variable chosen in the first step of the model, so their presence is redundant for the analysis. The strong association between size of silt/clay fraction and benthic community is well known and established (Manninom and Montagna, 1997, Engle and Summers, 1998, McRae *et al*., 1998, Borja *et al*., 2000). Gravel percentages are not only correlated with FF but also have a large standard deviation in each community's type (see Table 9.2). For these reasons Sand and Gravel variables were not used as input variables in later models.

Table 9.3 – Results of forward stepwise discriminant analyses conducted for combining the physical and chemical variables into the BI_{bio}. The Wilk's Lambda (0 perfect discrimination to 1 no discrimination), F statistics and their p values are given first for the overall model, then after elimination of the respective variable. The percentages of locations, which were correctly classified in the predictive and validation sub-sets, are also listed.

				Correct classifications (%)							
Variables included in the analysis	Wilk's Lambda	F	p	A1	B1	I	II	B2b	A2	B2a	Total
Model I	0.202	4.261	<0.000	Prediction dataset (validation dataset)							
FF	0.256	3.476	0.004								
Flow	0.263	3.954	0.002								
Shear stress	0.258	3.606	0.003	66.7	45.5	46.2	77.8	33.3	0	76.7	58.24
Velocity	0.252	3.241	0.007	(75.0)	(22.2)	(0)	(100)	(0)	(0)	(92.3)	(52.5)
Depth	0.220	1.125	0.356								
TOM	0.218	1.019	0.419								
Model II	0.217	5.860	<0.000	Prediction dataset (validation dataset)							
FF	0.257	3.343	0.014								
Flow	0.283	5.537	0.0006								
Shear stress	0.284	5.606	0.0005	66.7	50.0	46.2	77.8	-	-	76.7	63.9
Velocity	0.274	4.790	0.0017	(75.0)	(33.3)	(50)	(75)			(84.6)	(63.9)
Depth	0.233	1.280	0.286								
TOM	0.232	1.267	0.291								
Model III	0.232	6.817	<0.000	Prediction dataset (validation dataset)							
FF	0.366	10.678	0.0000								
Flow	0.305	5.846	0.0004	66.7	54.5	30.8	77.8	-	-	70.0	60.2
Shear stress	0.303	5.666	0.0005	(75.0)	(44.4)	(33.3)	(100.0)			(76.9)	(63.9)
Velocity	0.295	4.981	0.0013								
Depth	0.247	1.211	0.3131								

Model I has a total percentage of correct classification (hit ratio) of 58 % in the prediction sub-set and 53 % in the validation sub-set. According to the maximum chance criterion (C_{max}) the highest probability of occurrence of correct classification by chance would be 34 % and according to the proportional chance criterion (C_{pro}) this percentage would be 21 %. Since C_{max} is greater than C_{pro}, the maximum chance criterion is the one to outperform. The hit ratio for the validation set exceeds C_{max} criterion, so the discriminant model was considered valid. However the percentage of correct classification in the predictive and validation sub-sets was 0 % for community A_2 (Table 9.3). This community was only found at 8 stations in the total data set, and the physical and chemical parameters of this community's small areas have a larger variance and are far from the gradient of organic load enrichment found from *marine type* to *estuarine disturb*ed communities (Table 9.2). In addition, the community B_{2b} although with a hit ratio of 33 %, does not have any correctly classified station in the validation sub-set (Table 9.3). This community looks reasonably defined by the physical and chemical parameters (Table 9.2), but it was only found in 4 stations (Fig. 9.1) which makes their prediction unreliable. A 50/50 proportion for the prediction and validation sub-sets was also investigated and it led similarly to a 0% of correct classifications for A_2 and B_{2b}. Even when using the whole dataset (131 sampling points) the misclassification rate for A_2 was 100%, although for B_{2b} 100 % of locations were correctly classified. For the reasons explained earlier the communities A_2 and B_{2b} were not included in later models. Using fewer communities in the SDA will lead to a loss of information by the Index but a gain in its prediction accuracy (Degraer *et al.,* 2002).

Model II was computed without A_2 and B_{2b} communities and Sand and Gravel variable. The total hit ratio improved not only in the predictive (63.9 %) but also in the validation datasets (63.9 %) (Table 9.3). These values exceed C_{max} and C*prop* (36 % and 25 %, respectively for 5 groups).

In both Models I and II, TOM and Depth variables contribute little to the discriminatory power of the model (see Table 9.3, *p* values higher than 0.05) and were the last variables to enter the model. TOM variable is strongly correlated with Fine fraction (0.90) and significantly correlated with all the other variables. Depth variable although significantly correlated with most of the variables, have lower correlation values (Table 9.4).

Table 9.4 – Pearson correlations between the physical and chemical variables. Significant correlations ($p < 0.05$) marked with *.

	FF	Sand	Gravel	TOM	Shear St.	Flow	Velocity	Depth
FF	1.00	-0.98*	-0.32*	0.90	-0.50*	-0.41*	-0.44*	-0.32*
Sand	-0.98*	1.00	0.10	-0.88	0.50*	0.38*	0.46*	0.23*
Gravel	-0.32*	0.10	1.00	-0.31	0.11	0.25*	0.03	0.46*
TOM	0.90*	-0.88*	-0.31*	1.00	-0.53*	-0.41*	-0.49*	-0.31*
Shear St.	-0.50*	0.50*	0.11	-0.53	1.00	0.61*	0.94*	0.17
Flow	-0.41*	0.38*	0.25*	-0.41	0.61*	1.00	0.69*	0.60*
Velocity	-0.44*	0.46*	0.03	-0.49	0.94*	0.69*	1.00	0.22*
Depth	-0.32*	0.23*	0.46*	-0.31	0.17	0.60*	0.22*	1.00

In Model III, Sand, Gravel and TOM were not included and the hit ratio of the prediction sub-set (60.2) is slightly less than Model II, but higher than for Model I. Nevertheless the percentage of correct classification in the validation sub-set equals the one obtained for Model

II (63.9 %) (Table 9.3).

When using prediction and validation sub-sets of equal size the hit ratio of Model II is 64.5 % for the prediction sub-set and 58 % for the validation sub-set (compared to a prediction of 58.8% and a validation of 50.7 % in Model I). Again with sub-set 50-50 and not including Sand, Gravel and TOM (Model III), the model decrease the hit ratio (56.5 %) in the prediction sub-set and has a hit ratio of 61.4 % in the validation sub-set.

Model II agrees with natural conditions and other studies. Associations between organic matter and benthic communities are largely reported (Manninom and Montagna, 1997, Bakri and Kittaneh 1998, McRae *et al.*, 1998). Snelgrove and Butman (1994), suggested that the amount of hydrodynamic energy and available organic material are more likely to be primary driving forces, with depth and sediment grain size as secondary correlates. Rees *et al.* (1999), also found that tidal current velocity, depth and sediment type help to explain the distribution of benthic assemblages. Although the hydrodynamic energy is difficult to measure in the field, the use of 3D hydrodynamic simulation models allows the prediction of these parameters at any instant or averaged over any period of time (Martins *et al.,* 2001).

In conclusion, Model II provides better prediction since it is the model for which fewer variables are discarded (2 instead of 3 for model III) and 2 groups with poor classification scores are removed. To test this model the samples belonging to groups A_2 and B_{2b} (which were eliminated from the validation dataset) were used as validation sets. For the locations belonging to community A_2 the model classified them in 4 types of different communities (A_1 – 12.5 %; B_1 – 25 %; B_{2a} – 50 %, II 12.5 %). The high variance found for the physical and chemical parameters of these stations explains the extent of their misclassification. For the locations belonging to community B_{2b}, the model classifies 50 % in community I and the other 50 % in community II. Those communities are the ones nearest to community B_{2b}.

The classification functions of Model II used for Benthic Index calculation are listed in Table 9.5.

9.3.2 Benthic biotopes prediction

BI_{bio} index was calculated at the 77 sampling points using the classification functions of Model II (Table 9.5) and then eq. 9.3. Results by station and by management unit are shown in Fig. 9.2. In Annex VIII (Table VIII.1) are listed the parameters introduced in the model and

Index results in the 77 points. The benthic communities were classified in 1 to 1.4 – Marine; 1.5 to 2.4 – Transition; 2.5 to 3.4 – Estuarine; 3.5 to 4.4 – Estuarine enriched; 4.5 to 5 – Estuarine impoverished.

The model selected first the variable FF and the benthic index is significantly correlated with it (r^2 = 0.66). As stressed earlier, sediment grain size is an important factor for benthic composition. Since a more densely sampled dataset is available for the same study area and period of time (153 sampling points Caeiro *et al.,* 2003a – Chapter 4), BI_{bio} was interpolated using co-kriging and FF used as secondary variable. Co-kriging helps reducing the variance of the estimation errors wherever the variable of interest is under sampled and well correlated with the secondary variable (Isaaks and Srivastava, 1989). For BI_{bio} a geometric anisotropy semivariogram model was fitted visually to capture the longer range in the direction of azimuth 120º that corresponds to the water flow*.

Table 9.5 – Classification functions (W_j) for each community z of Model II for BI_{bio} calculation.

Variable (j)	Marine Type (A_1)	Transition region (B_1)	Estuarine type (B_{2a})	Estuarine impoverished (I)	Estuarine enriched (II)
FF	-1.68786	-1.62273	0.74695	-0.32941	3.22446
Flow	3.42315	-0.15635	-0.55361	-0.28041	-0.34494
Shear Stress	6.52528	-0.54224	-0.19505	-1.56882	-1.21969
Velocity	-6.15078	0.60679	0.63274	0.97355	0.38343
Depht	-0.58882	0.56611	-0.09986	-0.09487	-0.02608
TOM	-0.13869	0.46169	-1.08579	0.94509	0.26584
Constant (C_z)	-6.87994	-1.81065	-1.20610	-2.24548	-5.26877

The spatial pattern of the BI_{bio} is similar to the spatial distribution of the benthic communities found by (Rodrigues and Quintino, 1993) (Fig. 9.1 and 9.3) although some differences are expected due to changes in the sediment characteristics (see FF spatial distribution in Fig. 9.4). The marine community characterized by clean sand sediments is found at the entrance of the estuary, but in comparison to the 1986 campaign, this community moved to the entrance of the North Channel replacing former transition communities. These changes were already noticed in a 1997 study conducted along the Entrance Channel and the Northern Channel (Rodrigues and Quintino, 2002). These authors stress that these changes are related to dredge operations and the resulting decrease in organic load. According to them this induces biodiversity loss, associated with inward spread of the open sea marine assemblage, which is

* Cross-validation procedures (see Annex IV) were computed to evaluate the impact of the semivariogram model on interpolation results.

less rich and abundant, and typical of coarser clean sands. The lower river flux entering into the estuary during the last decades can also explain these benthic changes.

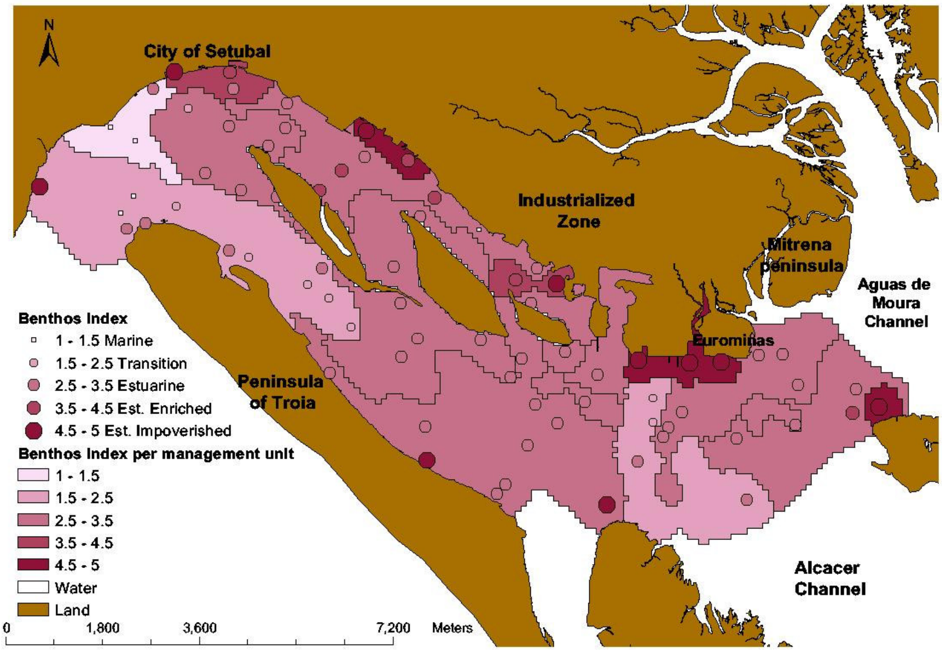

Figure 9.2 – Maps of the values of the index Bi_{bio} at sampled locations and averaged within management unit in the Sado Estuary.

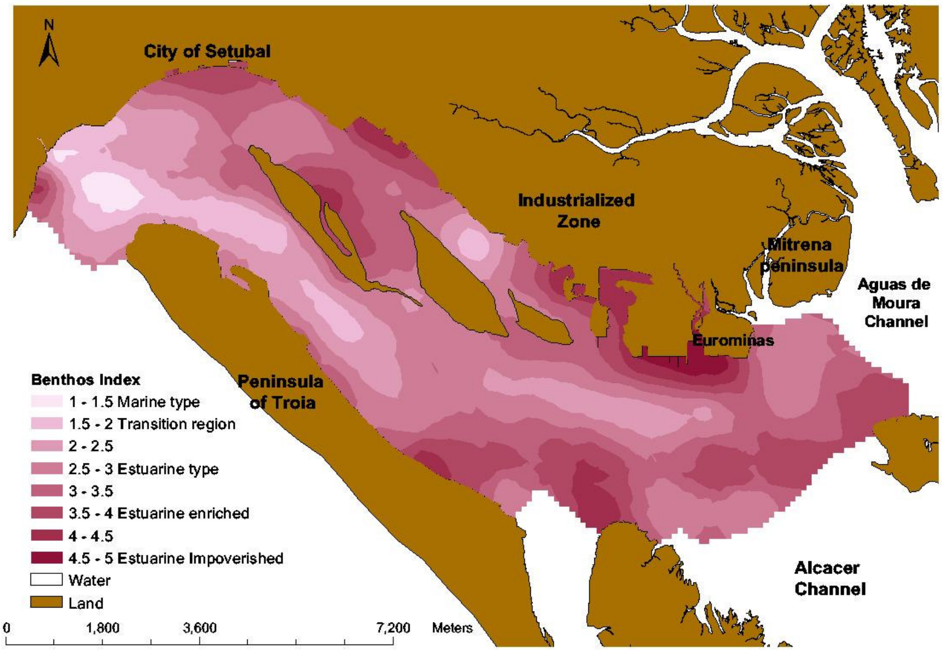

Figure 9.3 – Spatial distribution of the Bi_{bio} in Sado Estuary.

The transition region follows the marine type community, spreading over a large area more through the Southern Channel (Fig. 9.3). In comparison with the earlier spatial distribution of benthic assemblages (Rodrigues and Quintino, 1993) the transition regions seem to have spread to inner parts of the estuary, replacing a former small area of marine community existent near the sandbank (Fig. 9.1). In agreement with benthos sampling studies undertaken in the Southern Channel in 1999 (Carvalho *et al.*, 2001), changes involve an increase in abundance and species richness, associated to organic enriched areas. This enrichment is also illustrated by the presence of larger areas of estuarine enriched and impoverished communities near Eurominas industry, replacing the estuarine type community (Fig. 9.1 and 9.3).

The estuarine enriched and impoverished communities associated with higher organic load are located near the urban area of the city of Setúbal, and in small areas along the north margin, near industrial wastewater discharges. At the entrances of Águas de Moura and Alcácer Channels two sampling points have high levels of the Benthic Index (Fig. 9.2). These locations are associated with low hydrodynamics and low depths, so high organic loads (Fig. 9.4), and can also be related to non-point pollution runoff and deposition. These non-point sources could be due to aquacultures and rice fields' activities upstream of those channels. Most contaminants entering estuarine bodies of water become particle-bound (Alden *et al.*, 1997) and are eventually concentrated in fine-grained sediments, and most low-dissolved oxygen events occur over fine-grained bottoms (Diaz and Rosenberg, 1995).

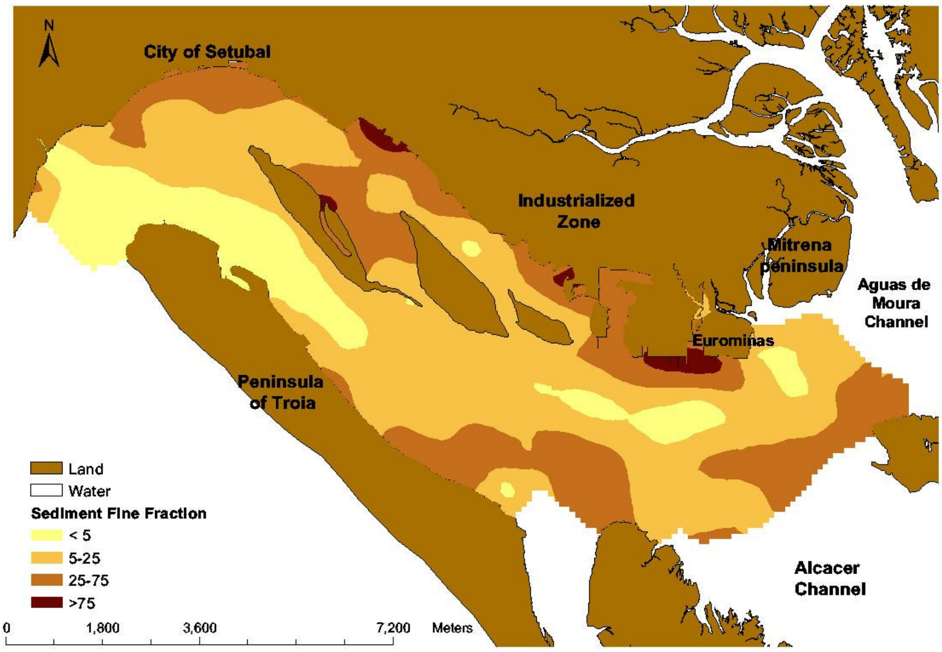

Figure 9.4 – Spatial distribution of sediment fine fraction (< 63 μm) in Sado Estuary.

Comparing the communities predicted in 2000/01 with the ones found in 1986, it can be noticed that both have a similar distribution (Fig. 9.5). However there was a decrease in the proportion of communities belonging to the transition region (species richness peak) balanced by a gain in the estuarine communities, resulting in a loss of biodiversity, as already stressed by (Rodrigues and Quintino, 2002).

The benthic biotopes gradient used in the BI_{bio} index was previous delineated for the Sado Estuary by other authors based on multivariate ordination analyses and relation with physical and chemical data. These multivariate methods have been found to be powerful tools for assessing perturbations to benthic in fauna assemblages (Smith *et al.*, 2001). Those gradients are in accordance with (Pearson and Rosenberg, 1978) that suggested that benthos respond sequentially to different levels of stress with species replacement occurring at the lowest level, and loss in diversity, abundance, and biomass occurring at increasingly higher levels of stress. These gradients have also been successfully incorporated in other benthic indices to allow the evaluation of their sensitivity to an increasing stress gradient (e.g. Majeed, 1987, Grall and Glémarec, 1997, Weisberg *et al.*, 1997, Borja *et al.,* 2000). Other studies developed a model that predicts solids accumulation on the seabed and associated changes in the benthic faunal community, using the Infauna Trophic Index. From quantitative relationships between benthic community descriptors and solids accumulation (including hydrodynamics and depth), the level of benthic community impact in marine cage farms was predicted (Cromey *et al.*, 2002). Also Degraer *et al.* (2002) demonstrated that knowledge of the physical and chemical environments can be used to predict the occurrence of the macrobenthos.

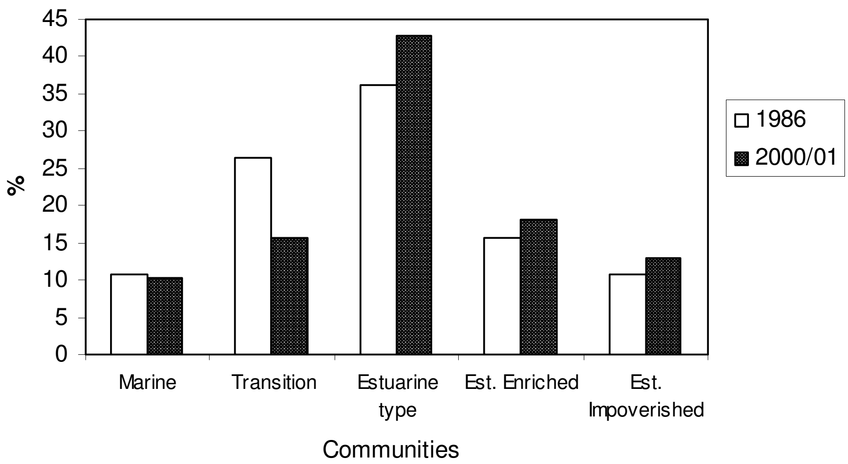

Figure 9.5 – Frequency distributions of the community types found in 1986 and the ones predicted in 2000/01.

Nevertheless, further testing and refinement of this Index should be done to allow a correct prediction of all type of communities found in the studied estuary and new data should be collected to validate this model. Also it should be tested in other estuarine ecosystems.

No single method is likely to produce stress classification without unacceptable misclassification. Ecological stress, from any source, is best measured by multiple methods or analysis under different assumptions. The consistency of classification obtained using different approaches would provide the robustness necessary to judge the reliability of a stress classification (Dauer, 1993). Combining the index with other measures of habitat quality, such as direct measures of sediment contamination and toxicity, can reduce misinterpretation of the data and provide a powerful weight-of-evidence approach to assessing the overall condition of a site, estuary or region (Van Dolah *et al.,* 1999).

The results of the index will be combined with contaminant and toxicity data representative of each management unit according to a Triad approach (Chapman, 1996). The sediment quality assessment of the management units will evaluate the *State* and *Impact* of the estuary according to the DPSIR indicators framework for data syntheses and management (Caeiro *et al.,* 2002 – Chapter 2). This framework is used to link social and economic pressures with environmental quality, making possible to formulate societal *Responses* that results in the formulation of an environmental policy.

9.4 CONCLUSIONS

Over the past two decades, indices of biological conditions have been adopted as tools for comprehensive monitoring of ambient water quality, and increasingly they are being incorporated into regulations in the form of numerical, biological criteria (Jacobson, 2000). The emphasis on benthic indices is appropriate because central to the assessment of a system's viability or health is the quality of its benthic habitats and the communities they support (Diaz *et al.,* 2003). Also they could be very helpful for estuaries quality compliance, namely according to the European Water Framework Directive. Benthic index are statistically precise, biologically meaningful and very cost effective (Roberts *et al*., 1998). Despite their limitations, they have been proven to be valuable tools for assessing sediment quality in a variety of estuarine habitats (Engle and Summers, 1999).

The problem with most of the benthic studies is the need of large databases and benthic community analyses data that are very time intensive to build and have often been criticized (Olsgard *et al.,* 1997). Several studies are exploring easier and less time consuming ways to analyze the benthic structure to assess pollution in macrobenthic community structure, such as the use of: i) acoustic and optical imaging, like side scan sonar images, multibeam echosounders or sediment profile images (Nilsson and Rosenberg, 1997, Cutter and Diaz, 2000, Santoro *et al*., 2002, Sutton *et al*., 2003) i) lower levels of taxonomic discrimination required to detect pollution: analysis at the phylum level (Warwick 1988a, Warwick 1988b, Warwick and Clarke 1993, Drake *et al.,* 1999), order level (Marqués *et al*., 2001) or family level (Warwick, 1988b, Costa, 1995, Olsgard *et al.,* 1997, Urkiaga-Alberdi *et al.,* 1999) and iii) trophodynamic groups classification (Mucha and Costa, 1999).

In this paper we presented an index methodology to predict the occurrence of macrobenthic communities, from physical and chemical variables such as sediment type, organic matter, depth and hydrodynamic parameters. This permits one to predict the occurrence of benthic biotopes at unsampled locations in a cost-effective way. The index allows concluding that the benthic distribution in the Sado Estuary is characterized at the entrance of the estuary by marine and transition communities, undisturbed and with high species richness. The transition region spreads over a large area through the Southern Channel. The more disturbed and organic enriched communities are found in the North Cannel, near industrialized areas, an in a small area at the entrance of Águas de Moura Channel. Comparing the benthic communities assessed 20 years ago it appears to have occurred a decrease of communities belonging to the transition region and a gain in the estuarine and more disturbed communities.

Although further testing is needed, using Bi_{bio} it was fairly easy to synthesize the ecological information required to visualize biotope gradients. This indice although not being a ready to use formula to apply in other estuarine systems, like other benthic index (e.g. Engles and Summer, 1999), their methodology can be applied elsewhere.

This type of index could also be combined with imaging techniques for bathymetric-sedimentological mapping. Once the most appropriate imaging technique for estuaries has been selected, it can be introduced as input data to the model. Those techniques statistically assess differences in benthic habitat quality and were already used in estuarine benthic studies (Diaz *et al*., 2003, Sutton *et al*., 2003).

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CHAPTER 10 – OPTIMIZATION OF SEDIMENT ESTUARINE MONITORING PROGRAM USING CONTAMINATION DATA

OPTIMIZATION OF SEDIMENT ESTUARINE MONITORING PROGRAM USING CONTAMINATION DATA

Caeiro, S., Nunes, L., Goovaerts, P., Painho, M. and Costa, M. H. (2003)
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ABSTRACT

This work develops the optimization selection of a subset of sediment monitoring sampling stations, based on a long campaign and data on contamination evaluation. The network thus obtained will be used as a long-term monitoring program to be integrated in an environmental and data management system for the Sado Estuary. Thirty stations were chosen to monitor management unit which are the basis of the management tool. This monitoring program represents a cost and technical benefit and it is assured that all the areas are sampled, including the stations with higher variability and contamination.

KEYWORD: sampling design; optimization procedure; long-term monitoring program

10.1 INTRODUCTION

Estuarine areas are usually highly populated and industrialized, which result in important pressures on the environment. These pressures may inflict severe negative environmental impacts if not carefully managed. It is then necessary to manage them in an integrated perspective, considering among other things the impact of activities discharging effluents into the estuary. The environmental management of these ecosystems cannot be conducted effectively without reliable information about changes in the environment and on the causes of those changes. Ecological monitoring programs represent an important source of that information. Monitoring should be planned in order to provide quantitative assessments of pollutants' complex effects. In particular this monitoring should be carefully designed in estuaries due to their high productivity, complex spatial variability and processes involved. Sampling designs that provide statistically unbiased estimates of the status, trends, and relationships, are then crucial.

The team has been working on the development of an environmental data management system through sediment quality assessment for the Sado Estuary (EMMSado) in the south of Portugal. In this management system the spatial and temporal data are integrated in a Geographical Information System, based in the DPSIR Model (Caeiro *et al.,* 2002 – Chapter 2).

The aim of this work is to select a subset of sediment monitoring sampling stations, based on a long campaign and data on sediment contamination. This network will be the base of a long-term monitoring program to be integrated in the EMMSado. This article comes in the sequence of two other where prior phases in the selection of the best location of monitoring stations for sediment quality were studied (Caeiro *et al.,* 2003b - Chapter 3 and Caeiro *et al.,* 2004 – Chapter 7).

10.2 METHODS

10.2.1 Previous work

Within the management system 19 spatially contiguous regions (management units) were delineated using a multivariate geostatistical analysis on sediment granulometry, organic mater content and redox potential (cluster analysis of dissimilarity matrix function of geographical separation followed by indicator kriging of the cluster data) from an extensive stratified random sampling campaign (153 stations) (Caeiro *et al.* 2003a – Chapter 4). The homogenous areas are the management units of the EMMSado. To avoid information redundancy as well as due to budget constraints, a smaller subset of the most representative stations was selected for contamination assessment according to organic load gradients (four groups). A monitoring network with 77 stations was obtained (Caeiro *et al.*, *2004* – Chapter 7). The resulting network was overlaid on the sediment management units previously defined using ArcGIS 8.1 GIS software (Figure 10.1).

All 77 samples were analyzed for the metals Cd, Cr, Cu, Hg, Pb, As and Zn. With this new information in hand a new optimization step was made: to select the best subset of stations out of the 77 that best represented the sediment quality and was therefore best suited for a long-term monitoring network. The number of stations in the subset was still to be determined. This optimization problem is a very difficult one because the number of possible combinations may attain very high numbers, making it impossible to evaluate all combinations exhaustively in a reasonable amount of time. Special algorithms are necessary to search for very good solutions in technically and economically times in such high dimensional combinatorial spaces. One of the algorithms that has been used with very good results is the simulated annealing algorithm (Kirkpatrick *et al.*, 1983, Cerny, 1985). It was also used to monitoring network optimization by Pardo-Igúzquiza (1998) and Nunes *et al.* (2002).

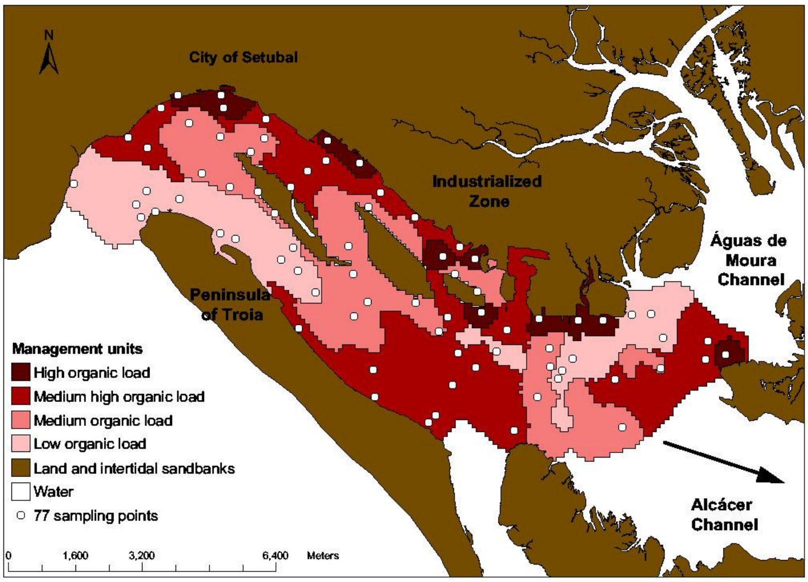

Figure 10.1 – Sado Estuary sediment sampling design overlaid on the sediment management units (Adapted from Caeiro *et al.,* 2003a – Chapter 4).

10.2.2 Special constraints

The new subset of stations, which will be identified as set *S''*, must reflect the sediment physical and chemical variability and spatial distribution detected with the exhaustive sampling campaign, and reflected in the original set of 77 stations (set *S'*). Therefore two constraints were imposed:

i) that the proportions of monitoring stations in the organic load groups in set *S''*be similar to the proportions in the original set, *S'*;

ii) that the proportions of an ecological risk index categories in set *S''* be similar to the proportions in set *S'*.

The main aim of the first constraint is to ensure the monitoring in all organic load groups, therefore keeping the constraint used in the works that preceded this article. Their calculations will be explained further on this text.

For the second constraint, the heavy metals data were summarized in an index of ecological risk – the mean Sediment Quality Guidelines-quotient (SQG-Q). This index works as a central tendency indicator of adverse biological effects owing to mixture of chemicals in different concentrations. The use of this type of numerical SQG-Q provide source of candidate chemical targets for assessing sediment chemical data (MacDonald *et al.,* 2000) and are very useful for a first screening of sediment contamination (Long and MacDonald, 1998, Chapman and Wang, 2001). Mean SQG-quotient was calculated for each sampling station α, using the following equations (Long and MacDonald, 1998):

$$SQG-Q_{\alpha} = \frac{\sum_{i=1}^{n} PEL-Q_{i\alpha}}{n} \qquad \text{(eq. 10.1)}$$

where:

$$PEL-Q_{\alpha} = \frac{C_{\alpha}}{PEL} \qquad \text{(eq. 10.2)}$$

PEL-Q - Probable effect level quotient for each contaminant *i*
C- Heavy metal concentration in each sampling station
PEL - Probable effect level of each contaminant *i*
n – number of contaminants used.

PEL is the concentration above which adverse effects frequently occur and was first calculated for the State of Florida (MacDonald *et al*., 1996) (Table 10.1). Their reliability and predictive ability indicate they can be used effectively to assess the quality of coastal sediments (Long and MacDonald, 1998).

Table 10.1 – Probable Effect Level of metals analyzed in this study (MacDonald *et al.,* 1996).

	Cd	**Pb**	**Zn**	**Cu**	**As**	**Cr**	**Hg**
PEL ($\mu g g^{-1}$)	4.21	112	271	108	41.6	160	0.7

According to MacDonald *et al.* (2000) a sampling station can be scored in three impact level categories:

Category 1: *SQG-Q* ≤ 0.1 unimpacted – lowest potential for observing adverse biological effects;

Category 2: 0.1< *SQG-Q* <1 impact – moderate potential for observing adverse biological effects;

Category 3: *SQG-Q* ≥ 1 highly impacted – potential for observing adverse biological effects

Both constraints are easily included in the optimization algorithm, but also make the search for new solutions more time consuming because more solutions have to be tested for compliance with the restrictions. Unfortunately there is no way to test a priori if a solution fulfils the constraints that is faster than by including it in the algorithm. Once again testing all solutions exhaustively before the optimization procedure would take an impossible amount of time.

10.2.3 Optimization model

Variance-based methods, also known as variance reduction methods, consider that the uncertainty associated with a given monitoring network may be determined by the variance of the estimation error obtained by kriging. The higher the variance the lower the accuracy. A given spatial distribution of stations has an uncertainty that depends on the particular locations. If one station is removed or another is added, the accuracy will usually decrease in the first case and increase on in the second. Also, if the number of stations is kept not changed, and only their location altered, accuracy will change. Mean squared estimation error is therefore used as an objective function.

The set of stations that produce the lowest mean squared estimation error result in a spatial distribution with the highest accuracy. The objective function considers a set, *S'*, of all the original stations, with cardinality *Ω'*, and take a subset, *S''*, with cardinality *ω'*, such that *ω'<Ω'*.

Minimize

$$s_K^2 = \frac{1}{\omega} \sum_{\alpha=1}^{\omega} \left[i(x_\alpha) - i^*(x_\alpha) \right]^2, \omega' \in S'', S'' \subset S' \qquad \text{(eq. 10.3)}$$

Subject to:

Constraints i) and ii)

s_K^2 is the mean squared estimation error, α indicates the station, and $i(x_\alpha)$ is an integer variable which takes four values, corresponding to four organic load groups: 1 for High Organic load (HO), 2 for Medium High (MHO), 3 for Medium (MO), and 4 for Low Organic load (LO) (Caeiro *et al.*, 2003a – Chapter 4), $i^*(x_\alpha)$ has the same meaning as $i(x_\alpha)$ but represents the estimated value, and x_α the location of station α.

10.2.4 Number of stations in the subset

There is still the need to define the number of stations in the new subset, *S''*. For such it was necessary to establish the maximum relative error when estimating the mean concentration with the new subset, that is the new monitoring network will have an assumed error which is lower or equal to *r* percent of the true mean with a given probability, γ. The equation for the number of stations, ω', is then given by (Cochran, 1977):

$$\omega' = \left(\frac{t_\gamma \cdot s}{r \cdot m}\right)^2 \Big/ \left[1 + \frac{1}{\Omega'}\left(\frac{t_\gamma \cdot s}{r \cdot m}\right)^2\right] \qquad \text{(eq. 10.4)}$$

where t_γ is the Student *t* statistical distribution value, *m* is the sample mean, and *s* its standard deviation.

The number of stations in each sediment management unit should be selected such that it is higher where the variance is higher, and lower where it is lower. This is common procedure called stratification which helps allocating more stations where they are most needed, but guaranteeing that a given total number of stations, ω', is not surpassed. The equation for proportional allocation can also be found in Cochran (1977):

$$\omega_l' = \omega' \cdot \frac{W_l \cdot s_l}{\Sigma W_l \cdot s_l} \qquad \text{(eq. 10.5)}$$

where s_l is the standard deviation in each management unit (stratum), W_l is the fraction of stations in the original set that were sampled in each management unit *l*.

The proportional allocation ω_l' for each management unit, will them be used for constrain i).

10.2.5 Optimization algorithm

Simulated Annealing (SA) algorithm with the Metropolis iterative improvement procedure (Metropolis *et al.*, 1953) was then used to solve the optimization model. This procedure generalizes by incorporating controlled uphill steps (to worse solutions). The procedure states the following: consider one small random change in the system at a certain temperature (the control parameters *t* is usually termed temperature); the change in the objective function is ΔOF; if $\Delta OF \leq 0$, then the change in the system is accepted and the new configuration is used as the starting point in the next step; if $\Delta OF > 0$ then the probability that the change is accepted is determined by $P(\Delta OF) = exp(-\Delta OF/t)$; a random number uniformly distributed in the interval (0,1) is taken and compared with the former probability; if this number is lower than $P(\Delta OF)$ then the change is accepted. The SA algorithm runs in the following way: i) the system is *melted* at a high temperature (initial temperature, t_1); ii) the temperature is decreased gradually until the system *freezes* (no further OF change occurs); iii) at each iteration the Metropolis procedure is applied; iv) if any of the stopping criteria is reached the algorithm is stopped and the best solution found is presented. More detailed description of the algorithm may be found in any combinatorial optimization textbook. The objective function is in this case given by equation (eq. 10.3).

The algorithm includes the constraints i) and ii) but considers a slack by introducing an interval within which the constraints are still accepted. For instance in the case of constraint i) if the proportion is 0.3 and slack of 20% is considered, then the proportion varies between 0.24 and 0.36. This is a necessary step to allow the search escape from non-optimal solutions.

The algorithm was implemented in a specific computer code: program OPTIVAR (Nunes *et al.*, 2003).

10.2.6 Cost analysis

A complementary analysis of exploration costs of sediment quality assessment was also performed. A cost per sampling was computed based on the previous sampling campaign and laboratory analysis costs (adapted from official costs of the laboratories in Portugal

ControLab, lda. and Instituto do Ambiente): i) linear distance between sampling points (study area - 56 km^2); ii) boat velocity: 12,8 km/h; iii) hour of work per day: 5 h/day; iv) time for sampling: 40 min; v) Boat cost per day: 260 Euros; vi) Cost per total analysis: contaminant – 612.25 Euros; toxicology – 1050 (only in stations with Fine Fraction contents higher then 5 %); Benthos structure analysis – 450 Euros; parameters of general sediment characterization: 85 Euros (discount: 25 % from 20 to 50 stations, 30 % from 55 to 77 stations).

10.3 RESULTS AND DISCUSSION

10.3.1 Number of stations in the subset

The number of stations ω' in the new design (subset *S''*) was calculated with equations (10.4) and (eq. 10.5), considering Cadmium concentrations as the variable. Cadmium was chosen since it was the heavy metal with the highest number of stations exceeding the contaminant thresholds and higher variability (according to the Portuguese Law on heavy metals in dredged sediment – DR, 1995). The mean cadmium concentration value of all stations was m=1.982 $\mu g g^{-1}$ and the standard deviation s=1.93 $\mu g g^{-1}$. Thus with a $t_{\gamma=0.1}$=1.295 and r in between r=0.15 and r=0.2 (that is accepting an error when estimating the mean between 15% and 20%), the number of stations varies between 26 and 37. An intermediate value of ω' =30 was chosen by also including budgetary constraints.

The exploitation costs analysis (Fig. 10.2) showed that costs are always increasing since the cost of sediment quality assessment analyses has a high weight in the total cost. Thirty is a good number for this monitoring program since: i) each of the 19 management units could be sampled at least at one location or two in case of larger or with higher variability areas, ii) the cost represents a decrease of 60 % compared with the initial sampling campaign (77 stations); iii) the budget limit was respected.

Table 10.2 shows the standard deviation values and the number of stations for each organic load group. In the last line of the table are included the proportion of estimated number of stations according to equation (eq. 10.5). These values, ω_i'/ω', i=1,…4, were used as constraints, as presented in the Methods section, as constraint *i*).

Constraint i) differs from constraint ii) in that the first forces the algorithm to find solutions that include proportions of stations according to their organic load content, while in the second the variable is the *SQG-Q* index. The proportions of categories 1, 2 and 3 of the *SQG-Q* index obtained in the 77 stations were: 1) 0.298; 2) 0.676 and 3) 0.026. It was used for both constraints a slack varying from 30 to 40%.

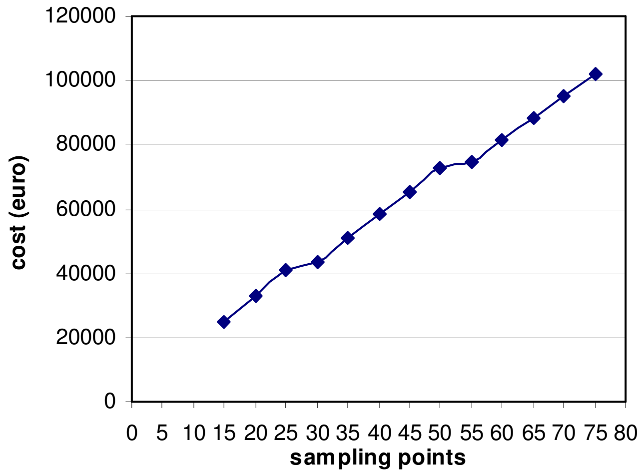

Figure 10.2 – Cost versus number of monitoring stations.

Table 10.2 – Standard deviation, samples per organic load group and ω_l'/ω', i=1,…4 (considering ω'=30).

	l			
	1 (HO)	2 (MHO)	3 (MO)	4 (LO)
s_l	1.997	1.448	0.401	0.335
Ω_l'	12	24	22	19
ω_l'/ω' (ω'=30)	0.324	0.470	0.120	0.086

10.3.2 Optimization results

Some first runs were performed letting the program choose a solution with 30 stations. Results showed that some constraints were not exactly observed, *e.g.*, ecological risk index category 3 was not always present in the solution found (only 2 stations belong to that category), as well as some management units were not sampled. Figure 10.3 indicates that with ω'=30 stations without additional constraints, not all the management units are sampled (three areas are not sampled). There was a high tendency not to choose stations in the areas belonging to the groups LO and MO. Since these groups have lower variance, a reduced proportion of estimated stations are required in the program (see Table 10.2). Even with ω=35 to 45 the solutions have at least one area that is not sampled. This was also a result of the slack included in the algorithm. Reducing the slack was not possible because the search would get easily trapped in non-optimal solutions. Without sampling those areas is not possible to assess and monitor their sediment quality and further define management actions to those areas. An alternative approach was used: i) a solution with 27 stations was searched; ii) this solution was set as additional constraint and three new stations were added by the program after searching in the unsampled areas (those management units belonging to organic load content classes 3 and 4). The results are depicted in Figure 10.4.

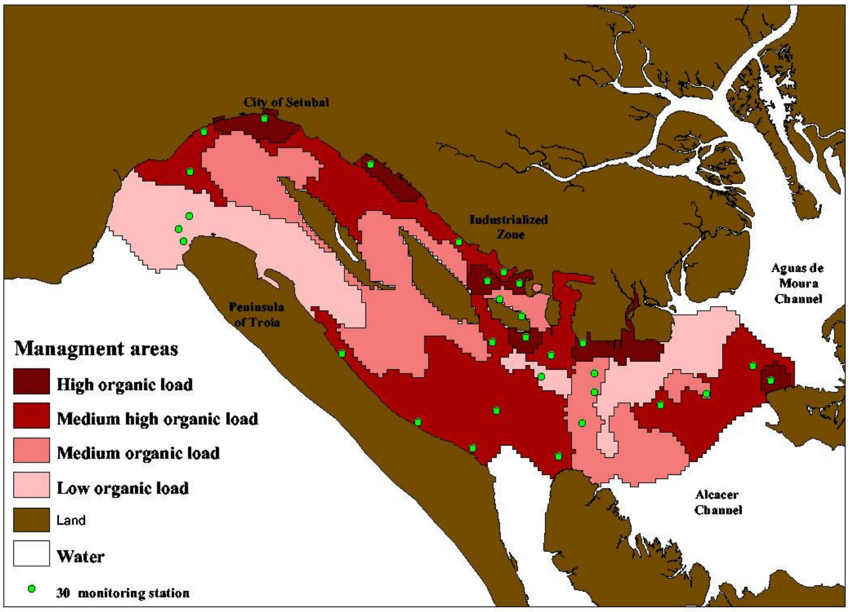

Figure 10.3 – 30 stations monitoring network without additional constraints.

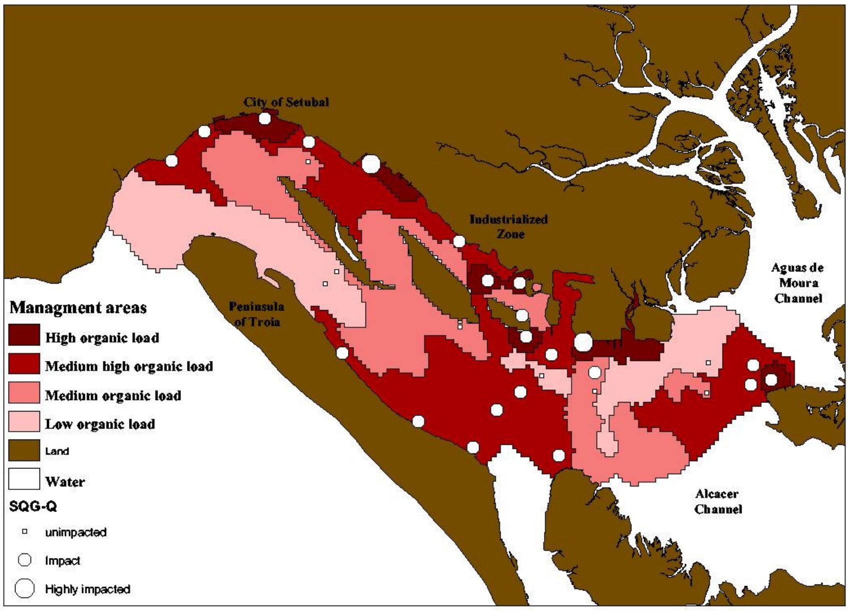

Figure 10.4 – Final monitoring network and scores of the ecological risk index.

10.4 CONCLUSIONS

This monitoring program represents an estimation error variance of 0.542, but a higher number of stations will be too time and cost consuming for a long-term monitoring program. Nevertheless with these 30 stations it is assured that all the areas are sampled and that the stations with higher variability and contamination are sampled in more detailed.

This monitoring network will be used to quantify and integrate the other two components essential to evaluate the sediment quality in each management units: toxicity and assessments of resident benthic community alteration (Chapman, 1996). The sediment quality assessment will then be integrated in the GIS with the social and economical pressures for the management delineation. It will also be used for future long-term monitoring of the management units for measuring the general state of the environment and to ensure that environmental components is not altered by human activity beyond a specific standard or regulating level.

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CHAPTER 11 – WEIGHT OF EVIDENCE TO ASSESS SEDIMENT QUALITY IN MANAGEMENT UNITS: APPLICATION TO THE SADO ESTUARY, PORTUGAL

WEIGHT OF EVIDENCE TO ASSESS SEDIMENT QUALITY IN MANAGEMENT UNITS: APPLICATION TO SADO ESTUARY, PORTUGAL

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(paper in preparation)

ABSTRACT

Sediments have been widely used to identify sources of contamination, to measure their extent, and to diagnose the environmental quality of estuarine ecosystems. The Sado Estuary in Portugal is a good example where it's urgent to perform a global sediment quality assessment, integrated with the diverse and intense human activities that take place in it. The aim of this work was to assess the quality of the sediment in environmental management units of the Sado Estuary. To evaluate the environmental significance of sediment contamination, an integrative burden-of-evidence approach was used, the Sediment Quality Triad, involving assessment of sediment chemistry, sediment toxicity and benthic community structure. The basis for decision-making for overall assessment was a statistical multivariate analysis incorporated into score matrix tables, using a Best Professional Judgment. This information was integrated and linked with the human *Driving Forces* and *Pressures* according to data management framework developed for Sado Estuary. From the nineteen areas analyzed, three of them presented no risk (18.5 % of the study area) and another, representing 5.6 % of the study area, are areas with high risk to cause adverse effects in the biota. These later areas, of high or medium high organic load, are located in the North Channel and suffer high human pressure mainly owing to industrial activities. Moreover, they also have low hydrodynamics, thus are associated with high levels of deposition. From the contaminants analyzed, the ones of concern are Cd, Cu, Zn, As, δ-BHC, Heptachlor, Isodrin, DDT and metabolits, Endosulfan and Endrin. Other important contaminants, PCB and PAH, should be measured on the study area to complement the Weigh of Evidence approach, since unmeasured chemical area causing adverse effects in some of the areas.

KEYWORDS: Sediment quality assessment, Weigh of Evidence approach, multivariate

analysis, Sediment quality Triad.

11.1 INTRODUCTION

It has long been recognized that sediments accumulate persistent and toxic chemicals, therefore contaminated sediments continue to be a major concern to regulators, managers and the public.

The use of Sediment Quality Values or Guidelines (SQG) alone may be sufficient for decision-making, but in some situations multiple Lines of Evidence (LOE) developed from sediment chemistry, toxicity and benthic community assessment, should be used to support sediment management decisions (McCauley *et al.,* 2000, Chapman *et al.,* 2002). A scientifically defensible Weigh of Evidence (WOE) approach is the appropriate framework in which to place the results from multiple LOE to provide a meaningful interpretation of ecological significance and to make sound management decision (Wenning and Ingersoll, 2002).

One of the first WOE approaches to marine pollution assessment is the Sediment Quality Triad (SQT) (Long and Chapman, 1985, Chapman *et al.,* 2002). Major advances have been made in gathering and assessing the different components of the SQT: sediment chemistry, toxicity and benthic community structure (Long and Chapman, 1985). However, a key issue remains the integrated use of such information for informed and realistic decision-making, including determining when sufficient data has been gathered to allow for a decision. Such integration should involve some level of subjectivity that means Best Professional Judgment – BPJ to address the complexity of ecological system and the limitation of field and laboratory investigations (Burton *et al.,* 2002a, Chapman *et al.,* 2002, Preston, 2002). Formalized use of WOE in the environmental sciences is relatively recent. The first formalized WOE framework for contaminated sediments, SQT, was based only in summary indices, where the stations values were divided by the ones of the reference stations (Long and Chapman, 1985). However the single use of these indices result in information compressions that can negate full use of WOE (Chapman *et al.,* 2002), since they do not allow to highlight multi associations between the different contaminants and the adverse effects.

Although there is no “one-size-fits-all” the basis for decision-making should be statistical multivariate analyses incorporated into logic systems. BPJ will always be necessary, and scoring systems can assist the logic systems. Such a sound basis for decision-making is particularly important for sites background contamination/effects, variable substrate types and complex contamination patterns, all of which increase the complexity of the analyses and create potential for confounding effects (Chapman *et al.,* 2002). The tabular decision matrix, a mean to assess sediment quality WOE (Chapman, 1990) remains an effective basis (a logic system) for sediment management decision-making (Burton *et al.*, 2002a, Chapman *et al.,* 2002). Tabular decision matrices can reasonably incorporate a limited level of ordinal response (ranked from 1 to 3 or 4 rather than simply plus or minus), but should emphasize a strong quantitative evaluation within LOE (like statistical summarization) prior to merging into the more qualitative matrix table (Chapman *et al.,* 2002). Carr *et al.* (1996) and Grapentine *et al* (2002) used a ranking procedure summing the LOE allowing the comparison and classification among stations. MacDonald *et al.* (2000) also used a ranking to classify sediment management units. An tabular ranking approach can be moderately robust, has moderate methodology but high degrees of sensitivity, appropriateness/applicability and transparency (Burton *et al.,* 2002b).

Weight-of evident is sometimes used as an approach for combining the information, however it is rarely used in a quantitative and statistical manner (Smith *et al.,* 2001). But quantitative approaches although having several strengths are too complex (Burton *et al.,* 2002b) and difficult to understand by decision-makers.

Integration of different LOE should be done so that it draws on a broad range of interdisciplinary expertise (from stakeholder to scientific experts) to encompass the primary exposure and effects linkages. This then allows an interdisciplinary team to combine the LOE into a WOE matrix table for the decision making process (Burton *et al.,* 2002a). These consensus-based WOE approaches describe an open, multi-stakeholder process that ranges from qualitative to quantitative. Incorporation of more quantitative linkages of the various LOE with consensus-based approaches (e.g. Grapentine *et al.,* 2002) moves the scientific-decision making process forwards and improves our ability to both determine significant impairment to ecosystems and to respond appropriately (Burton *et al*., 2002b).

The aim of this work is to assess the quality of the sediment in environmental management units (areas) of the Sado Estuary. To evaluate the environmental significance of sediment contamination an integrative, burden-of-evidence approach was used, SQT, involving assessment of sediment chemistry, sediment toxicity and benthic community structure

(Chapman *et al.,* 1987; Chapman, 1990, Chapman *et al.,* 1996, Chapman *et al.,* 2002). The basis for decision-making, for overall assessment, was statistical multivariate analysis incorporated into logic systems. This information was integrated and linked with the human *Driving force* and *Pressures* in agreement with a data management framework developed for the Sado Estuary (Caeiro *et al.,* 2002 – Chapter 2). This tool is based on the indicator conceptual model DPSIR– *Driving forces, Pressures, State, Impact, Responses* (RIVM, 1995), where the SQT represent the *State* and *Impact* evaluation. This integration is according to the WOE Framework developed by (Burton *et al.,* 2002a). The management units (19) were delineated based on sediment parameters like Fine Fraction contents (FF), Total Organic Matter (TOM) and Redox Potential (Eh), measured in an extensive and appropriate sampling design and using multivariate geostatistical tools. Those units were classified in 4 types according to enriched levels of organic load (Caeiro *et al*. 2003b - Chapter 4) (Fig. 11.1).

11.2 METHODS

11.2.1 Study area

The Sado Estuary is the second largest in Portugal with an area of approximately 24,000 ha. It is located in the West Coast of Portugal. Most of the estuary is classified as a Natural Reserve but also with an important role in the local and national economy. There are many industries mainly on the northern margin of the estuary. Furthermore the harbor-associated activities and the city of Setúbal along with the copper mines on the Sado watershed use the estuary for waste disposal purpose without suitable treatment. In other areas around the estuary intensive farming, mostly rice fields, and also tomatoes, are the main land use together with traditional salt-pans and increasingly intensive fish farms (Caeiro *et al.*, 2002).

The Sado Estuary is characterized by a North Channel with weak residual currents, flow and shear stress, that enhance accumulation of sediment allowing locally introduced pollutants to settle down rather than be carried away. The southern channel, separated by the North Channel by sandbanks, is highly dynamic and tides are the main responsible for the water circulation. Geometric characteristics distinguish the outer estuary (our study area) from the inner estuary, corresponding to a narrow channel (Alcácel channel). The inner part of the outer estuary, (entrances of Águas de Moura and Alcácer Channels), is quite shallow with large tidal flats (Neves, 1985).

11.2.2 Sediment sampling

A sampling survey of seventy-seven locations was designed using an optimisation model to select the appropriate spatial distribution within the study area and in each management unit type based on a first extensive campaign sampled from October 2000 to January 2001 –153 locations (Caeiro *et al.,* 2004b – Chapter 7). According to Burton *et al.,* (2002a) the selection of adequate sampling sites and numbers of samples must ensure adequate statistical power to detect pre-defined biologically significant changes in responses and spatial characterization. On this seventy-seven locations parameters of sediment general characterization and heavy metals and metalloid were measured. The same optimization model was used to select the subset of stations that best represented the management units based on the seventhly-seven locations and the heavy metal and metalloids data (Caeiro *et al.,* 2003c – Chapter 10). The model chose thirty sampling points but owing to budget and logistic reasons, from the thirty stations, only in nineteen locations bioassays were conducted and pesticides measured, representing the worst scenario of each management unit. These nineteen stations campaign (second campaign) occurred from July to October 2003. In the field the sampling criterion was a compromise between the Global Position System-receiver (Garmin GPS 12xL) coordinates and reach the sediment type for the corresponding management unit. At each location, three replicates were taken with a Petit Ponar grab in the first campaign and with a Van Veen in the second campaign, and a composite sediment sample was formed.

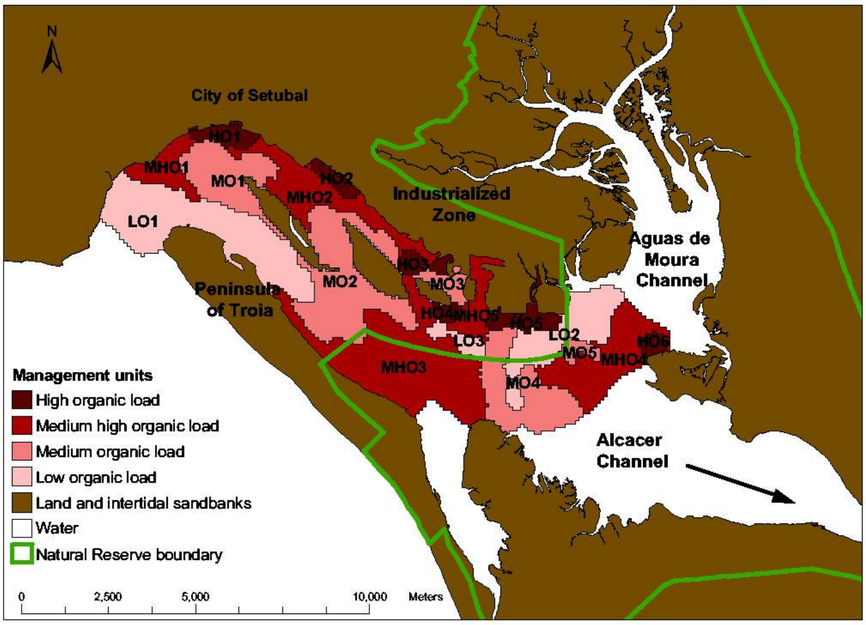


Figure 11.1 – Nineteen Management units of Sado Estuary and Natural reserve boundary. Adapted from (Caeiro *et al.,* 2003b – Chapter 4).

11.2.3 Sediment chemistry

A set of heavy metals and metalloids, Cd, Cu, Pb, Cr, Hg, Al, Zn and As, were determined using as analytical technique, Inductively Coupled Plasma Atomic Emission Spectroscopy. These contaminants are the more important heavy metals and metalloids, taking into account earlier work conducted in the estuary and estuarine pollution sources. TOM, FF, sand and gravel contents, and Eh were also determined for each location (Caeiro et al. 2003b – Chapter 4). The values of these parameters were calculated in each management unit using the median values of locations belonging to each unit (Caeiro *et al.,* 2003a – Chapter 8).

The following organochlorine pesticides were also determined: aldrin, dieldrin, pp' DDD, pp' DDE, pp' DDT, endosulfan I, endosulfan II, endrine, heptachlor, heptachlor epoxide, α-BHC, γ- BHC, δ-BHC. The organochlorine pesticides are of major concern due to their wide human use, persistence and bioaccumulation (Laws, 1993). They are rather stable compounds that tend to accumulate in lipid tissue and may persist long enough to be transported by run-off from atmospheric deposition and erosion of soils contaminated from past use. After run-off they easily sorb to organic material in sediment due to their hydrophobicity and persistence (Nowell *et al.,* 1999). Because of their persistence, organochlorine pesticides tend to be associated with biomagnification and food chains transfer problem (French, 1997). The sediment samples for pesticides were Soxhlet extracted with a mixture of hexane/acetone 1:1 for 10 h. Sulphur was eliminated with copper. The extract was filtered and concentrated in rotative evaporator at 50ºC until a volume of about 20 ml and concentrated in Nitrogen flow until a final volume of 1 ml. This extract was filtered over activated carbon for removal of colored impurities. The adsorbent was washed with 5 ml of hexane and 5 ml of acetone. The filtrate and the washing solvents were concentrated in nitrogen flow until a final volume of 3 ml. Analysis was performed on a gas chromatograph equipped with an electronic capture detector and a capillary column (DB608). Calibration and peak identification were performed using standard solutions containing the analyzed pesticides in a range of 5 ppb to 100 ppb. The recoveries of the concentration and clean-up steps were evaluated at the 30 ppb level and the final results were corrected with the respective recoveries.

The average Sediment Quality Guideline Quotients (SQG-Q) (Long and MacDonald, 1998) was calculated separately for heavy metals and metalloid, and pesticides using probable Effect Level (PEL) for each contaminant (Macdonald *et al.*, 1996). A classification of potential impact to cause adverse effects was performed according to (MacDonald *et al.*, 2000). For organic compound only the pesticides where PEL values were available were used (γ-BHC, p,p'-DDE, Dieldrin, p,p´-DDD and p,p'-DDT).

11.2.4 Sediment benthos structure

A benthic biotope index (BI_{bio}) was calculated in the seventy-seven sampling points. The values of the index in each management unit were calculated using the median values of the locations belonging to each management area. This Index predicts the occurrence of macrobenthic communities from physical and chemical variables, such as sediment type, organic matter, depth and hydrodynamic parameters. These parameters were measured, or simulated in the case of the hydrodynamic ones, at the seventy-seven sampling sites (Caeiro *et al.*, unpublished data – see Chapter 9). The macrobenthic communities data used was earlier delineated by other authors based on multivariate methods (Rodrigues and Quintino 1993). The index was computed through a discriminant analysis and the index varies from 1 to 5 and according to a stress gradient. The benthos communities were classified in:

1 to 1.4 – Marine;
1.5 to 2.4 – Transition;
2.5 to 3.4 – Estuarine;
3.5 to 4.4 – Estuarine enriched;
4.5 to 5 – Estuarine impoverished.

11.2.5 Sediment toxicity testing

Two toxicity bioassays were performed in whole and elutriate sediment in the 19 sampling points representative of each management unit. One of the bioassay was an acute test with mortality as the endpoint (10 days) with juveniles of marine amphipod *Gammarus locusta* from a laboratory standard culturing according to the procedure of Costa *et al.* (1998). This amphipod is an European species particularly abundant in Sado Estuary sensitive to sediment contamination, tolerant to a broad spectrum of sediment types and with excellent amenability for experimentation (Costa *et al.,* 1998). The other bioassay was conducted in the sediment elutriate with embryos of the Atlantic sea urchin *Paracentrotus lividus.* The toxicity was based on abnormal larvae development (72 h) and according to Rolland *et al.* (1999) and USEPA (1992) procedure. This bioassay is easy, fast and recommended for a regular bioassay for biomonitoring and environmental quality assessment and regulatory purpose (Rolland *et* *al.,* 1999, Beiras *et al.*, 2003). According to Chapman and Wang (2001) salinity could be a potential confounding factor when using marine species in estuarine sediment bioassays. However owing to low range of salinity in the study area (from 29 to 37 ‰ Rodrigues and Quintino, 1993) this confounding factor was not expected.

Management unit LO1 was considered the reference area, since this area has high hydrodynamics, is directly connected to the ocean and has no direct effluent disposal (Fig. 11.1). The baseline concentrations of the heavy metals found in this area are in accordance or are even lower compared to earlier data of Sado Estuary clean areas (e.g. Quevauviller *et al.*, 1989a).

11.2.6 Data analysis

One-tailed analysis of variance (ANOVA) followed by a Tukey test was computed in order to compare the sediments bioassays against the reference area (LO1) and the negative control (Zar, 1984). The negative control corresponds to the amphipods culture sediment and was obtained at the amphipod collection site; or the exposure of the eggs and larvae of sea urchin fertilized cell to seawater only. No reference control sediment was used for the amphipod bioassay since sediment type does not influence the bioassays results using these species (Costa *et al.,* 1998). In both bioassays the stations responses were corrected by the mean response in the negative control. Prior to ANOVA analysis the toxicity test data were tested according to requirements for normality and homogeneity of variance (Zar, 1984).

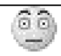
The data for SQT (chemicals, benthos and toxicity bioassays) were analysed using the multivariate statistical analysis Factor Analysis (FA) using the Principal Component Analysis (PCA) extraction procedure (with varimax normalized factor rotation) to explore variables distribution in accordance with DelValls and Chapman (1998), DelValls *et al.* (1999) and DelValls *et al.* (2002) procedure. This approach analyses potential multidimensional relationships between the values for chemical data and biological effects, and is followed by the classification of the samples into identified groups. The objective of PCA-factor is to derive a reduced number of new factors as linear combinations of the original variables, which will provide a description of the data structure with a minimum loss of information (DelValls and Chapman, 1998). The data was transformed (square root transformation in case of toxicity bioassays, $\log(x+1)$ for chemical and biotic index data and $\log(x+400)$ for Eh) to satisfy the test requirements for normality. The variables were standardized (centred and scaled) to be treated with equal importance.

Tabular Decision Matrix was used for WOE using the SQT first proposed by Chapman (1990), and improved by Chapman *et al.* (1996), Grapentine *et al.* (2002) and Chapman *et al.* (2002). Each Line of Evidence was judged on the basis of a graduation (a scoring system) to rate each measurement endpoint as indicative, moderate, or negligible/low ecological risk (Table 11.1). The LOE were summarized in SQG-Qs, toxicity bioassay results and Bi_{bio} index. The classification of the toxicity bioassay to use in the ordinal ranking scheme was based on ANOVA significant differences (value of p and tested the differences among the group of stations classified as low, moderate and high potential impact). The integration of data reducing techniques is very useful to use in Tabular matrix as stressed by Chapman (1996). Some legs of the SQT are assigned more weight than other, based on an expert knowledge of the sediment assessment, estuary behaviour and factor's interpretation computed from FA. The management unit type classification was taken into account, but only as a BPJ, to address the stability of surface contaminated sediment in accordance with Grapentine *et al.* (2002). According to these authors the stability of contaminated surface sediment must be assessed regardless of the local environmental impacts since a high-concentration point source may be a long-term source of contamination to areas downstream. Potential scenarios in which site stability could affect decisions about sediment quality and management should be identified.

The main *Driving Forces* (D) and *Pressures* (P) of each management type, including the potential main pollutants, were also integrated in the tabular analysis for overall judgment in accordance with DPSIR model. These items of the matrix take into account the human activities (D) that exert pressure (P) on the environment, causing changes on the state (S) and impacts (I) on the benthos ecosystem (Caeiro *et al.*, 2004a – Chapter 6). Their selection was based on the Sado Estuary data (e.g. Catarino *et al.,* 1987, AQUA/FCT/UNL 1997a, AQUA/FCT/UNL 1997b, Correia and Florêncio 2002), literature review (Laws, 1993, USEPA, 2001) and expert knowledge (Table 11.1).

Statistical analyses were conducted using Statistica® 6.0 software. To visualize and overlay the LOE results in the management units, within Coastal line of Sado Estuary, and *Driving Forces*/*Pressures* ArcGIS 8.0® GIS software was used.

Table 11.1 – Ordinal ranking scheme applied for weight of evidence categorization.

				
Chemistry	Metals and metalloid	• SQG-Q ≤0.1 (low potential impact for adverse effects)	• 1< SQG-Q < 0.1 (moderate potential impact for adverse effects)	• SQG-Q ≥ 1 (high potential impact for adverse effects)
	Pesticides	• SQG-Q ≤ 0.1 • (low potential impact for adverse effects)	• 1< SQG-Q < 0.1 • (moderate potential impact for adverse effects)	• SQG-Q ≥ 1 (high potential impact for adverse effects)
Toxicity	Amphipod mortality (whole sediment)	• No toxic (stations no statistically different from reference area p≥0.1)	• Moderate toxicity (stations statistically different from reference for $0.0001<p<0.1$)	• High toxic (stations statistically different from reference for p≤ 0.0001)
	Sea urchin larvae abnormality (elutriate sediment)	• No toxic (stations no statistically different from reference area p≥0.1)	• Moderate toxicity (stations statistically different from reference for $0.001<p<0.1$)	• High toxic (stations statistically different from reference for p≤ 0.001)
Benthos	Biotic index	• 1 – 2.5 (Marine and transition benthos assemblages)	• 2.6 – 4.5 (Estuarine type and enriched benthos assemblages)	• 4.5 – 5 (Estuarine Impoverish assemblages)
Management unit type		• *High organic load* management units were classified as "Stable"; *Medium organic load* and *Medium high organic load* management units were classified as "Medium Stable" and *Low organic load* management units were classified as "Unstable".		
Main Driving Forces/Pressure and Pressures components (potential pollutants)		• Defined for each management unit based on literature and expert knowledge.		
Overall Risk Assessment		• No significant adverse effects	• Potential significant adverse ecological effects	• High significant adverse ecological effects

11.3 RESULTS AND DISCUSSION

Results of the SQG-Q metals, SQG-Q pesticides, biotic index and toxicity bioassays per management unit are shown in Fig. 11.2.

None of the areas was classified with high chemical impact potential of adverse effects (Fig. 11.2 a and b). Metals index have areas with SQG-Q values near 1 and more areas classified as unimpacted compared with SQG-Q pesticide index. However it should be taken into account that SQG-Q for pesticides were only evaluated for the pesticides with available PEL values. All metals have similar spatial distribution and are mainly related with deposition areas near industrialized zones (e.g. near areas HO2, HO5)(Caeiro *et al.*, 2003a – Chapter 8). Pesticides showed different patterns. The areas LO2 and MHO4 at the entrance of Águas de Moura Channel have the highest impact potential according to SQG-Q pesticides index. Some management units have different classification levels of metals and pesticide SQG-Q indices, reflecting different contaminant sources (e.g. HO6, LO2 and HO4). These facts are further confirmed in the FA interpretation where the metals are all together in the same factor and appear only associated with two pesticides concentrations. The pesticides are spread over the different factors (Table 11.2).

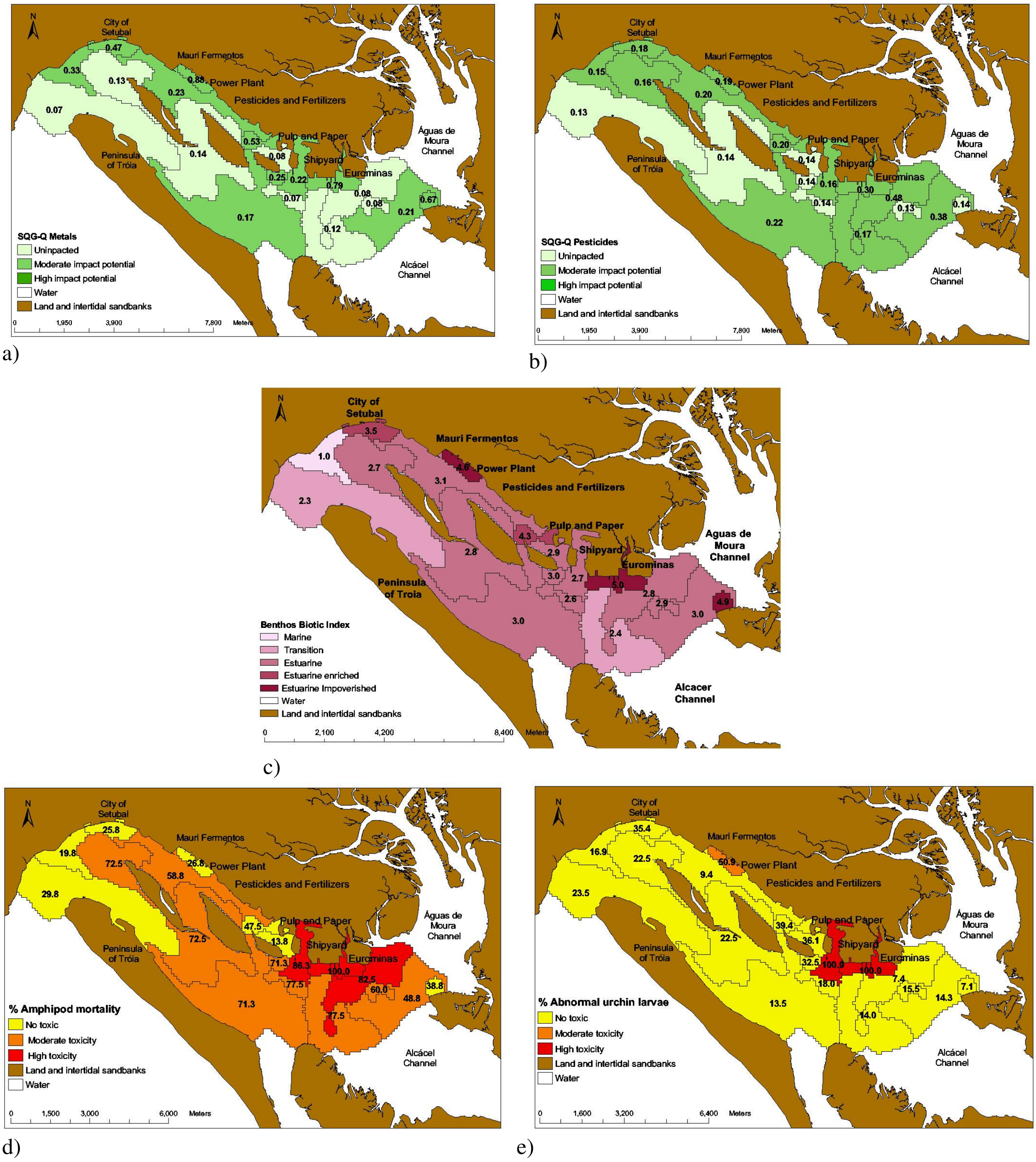


Figure 11.2 – a) Metals SQG-Q; b) Pesticides SQG-Q; c) Biotic index; d) amphipod toxicity bioassay and e) sea urchin larvae toxicity bioassay, in the Sado Estuary management units.

The *in situ* benthos alteration, evaluated through the biotic index showed clean and undisturbed communities at the entrance of the estuary, i.e. a marine type community at the north side of the estuary mouth and a transition region spreading over a large area through the Southern Channel. The more disturbed and organic enriched communities are found in the North Channel and in a small area at the entrance of Águas de Moura Channel (HO2, HO5 and HO6) (Fig. 11.2c).

Amphipods bioassay assigned more pessimistic scenarios when compared with the sea urchin larvae although in HO2 management unit it gave low toxicity results. This can be not only related with the high sensitivity of this amphipod species but also with higher levels of toxicity in sediment, associated with insoluble contaminant's forms (like the organochlorine pesticides), when compared with overlying water. Nevertheless in both bioassays the areas near pulp and paper industry and shipyard (MHO5 and HO5) at the North Channel correspond to sediments with high toxicity and the sediment areas at the entrance of the estuary, small area at the entrance of Águas de Moura Channel and HO3 and MO3 areas at the North Channel showed no toxicity (Fig. 11.2 d and e).

The factor analysis computed eight factors explaining 89.8 % of the total variance with the following interpretation (see factor loading in Table 11.2):

The first principal factor, is predominant and accounts for 44.7 % of the variance. This factor combines the chemical concentrations of the heavy metals and metalloid, the pesticides p,p´-DDE and p,p´-DDT, and organic carbon, fine fraction and sand and gravel (negative load) in sediment, the benthic index and the sea urchin bioassay (although with low load). It represents high biological effects associated with different chemical contamination and organically enriched sediment. Although some pesticides are included, the predominant group of contaminants are metals.

The second factor, explains 15.3 % of the variance. It combines the adverse effects measured by % abnormal sea urchin larvae with the sediment gravel (negative load) and the pesticides concentrations heptachlor, isodrin, p,p'-DDE (with higher load than in factor 1), p,p'-DDD, endrin and endossulfan II. A smaller contribution is also associated with Amphipod mortality (0.31) and benthos alteration (0.25). It represents high biological effects associated with pesticide contamination.

The third factor explains 8.0 % of the variance. It results on the combination of the negative loads of the contaminants γ-BHC, heptachlor epoxid and dieldrin with % abnormal sea urchin larvae. It represents the selected contaminants inversely associated with adverse biological effects, so individual levels of the analyzed contaminants do not explain toxicity.

The fourth factor explains 5.8 % of the variance. This factor in only associated with the pesticide endossulfan I. This contaminant is not associated with any adverse effects, therefore this pesticide is not bioavailable. Endolssulfan II and p,p´-DDT although having high loads, they are not as high as in the factors two and one, respectively.

Table 11.2 – Rotaded factor loadings from FA analysis. Loading >0.4 in bold.

Factor loadings	Factor 1	Factor 2	Factor 3	Factor 4	Factor 5	Factor 6	Factor 7	Factor 8
Amphipod (% mort.)	-0.234	0.309	-0.179	0.137	0.129	0.034	0.135	**-0.817**
Urchin (% abnormal)	0.286	**0.533**	**0.410**	-0.180	-0.217	0.241	0.018	-0.273
BI_{bio}	**0.514**	0.254	0.034	0.067	**0.544**	0.190	0.073	-0.214
Cd	**0.962**	0.182	0.089	-0.017	0.094	0.025	0.060	0.050
Pb	**0.932**	0.239	0.143	-0.070	-0.022	-0.003	0.030	0.026
Zn	**0.932**	0.171	0.057	0.052	0.095	0.016	0.097	-0.100
Cu	**0.966**	0.153	0.141	0.014	-0.026	0.090	0.089	0.015
Cr	**0.970**	0.120	0.096	0.048	-0.016	0.013	0.122	0.000
Hg	**0.889**	0.029	0.138	-0.082	0.173	0.169	-0.049	0.047
As	**0.937**	0.172	0.015	-0.045	0.218	0.045	-0.014	-0.027
TOM	**0.930**	0.156	0.130	0.089	0.003	-0.140	0.127	0.028
FF	**0.944**	0.133	0.131	0.098	0.006	-0.006	0.142	0.005
Sand	**-0.768**	-0.360	-0.062	0.044	*-0.407*	0.059	0.028	-0.073
Gravel	-0.376	**-0.465**	0.003	-0.178	*-0.681*	-0.058	0.163	0.001
Eh	-0.312	0.061	-0.094	0.022	0.042	0.025	**-0.903**	0.045
α-BHC	0.041	-0.116	-0.035	-0.053	0.101	**0.938**	-0.026	0.009
γ-BHC	-0.030	0.091	**-0.918**	-0.112	-0.158	0.038	0.066	0.052
Heptachlor	0.260	**0.832**	0.096	-0.097	0.029	-0.005	-0.056	-0.227
δ-BHC	0.356	-0.312	0.294	-0.174	**0.520**	0.296	0.114	0.136
Isodrin	0.117	**0.875**	-0.172	-0.061	0.133	-0.133	0.036	-0.077
Endossulfan I	0.003	-0.007	-0.024	**0.954**	-0.014	-0.068	-0.006	-0.054
Heptachlor epoxid	-0.350	-0.075	**-0.612**	-0.208	**0.497**	-0.096	-0.162	-0.190
p,p'-DDE	**0.488**	**0.767**	-0.002	0.243	0.026	-0.023	-0.058	0.056
Dieldrin	-0.277	-0.095	**-0.872**	0.150	0.012	0.042	-0.131	-0.109
p,p'-DDD	0.336	**0.548**	0.151	-0.041	-0.193	-0.196	-0.230	**-0.589**
Endrin	0.253	**0.924**	0.009	0.059	0.076	-0.031	0.002	-0.152
Endossulfan II	0.010	**0.747**	0.103	**0.588**	0.076	-0.045	0.029	0.004
p,p'-DDT	**0.612**	0.346	0.148	**0.471**	0.087	0.131	-0.164	-0.290

The fifths factor explains 5.6 % of the variance. This factor represents the combination of chemical concentration of the pesticides δ-BHC and Heptachlor epoxid, the benthic index and also the negative load of gravel and sand percentage in sediment. It represents biological effects associated with these pesticides contamination and related with sediments with low levels of coarser granulometry. Heptachlor epoxid have higher load in factor three, but it is negative.

The sixth factor explains 4.0 % of the variance. It results by the only contribution of α-BHC, not associated with any adverse effects, although precaution should be taken due to the sea urchin load (0.24).

The seventh factor explains 3.4 % of the variance and it represents the reduction conditions of the sediment, due to redox potential negative load.

The eighth factor explains 3.0 % of the variance. This factor represents the combination of negative loads of both p,p'-DDD concentrations and amphipod mortality, representing adverse effect associated with this pesticide but only when the management units have negative loads on this factor (see Fig. 11.3). This pesticide had already appeared associated with adverse effects in factor 1.

Because of the lower variance associated with factors 4 to 8 their interpretation must be regarded with caution and they were only included in the analysis to increase the overall total variance. For example p,p'-DDT and endolsulfan II appear associated with adverse effects in factor 1 and 2, but in factor 4 they are not associated with any adverse effects. Due to lower significance of factor 4 and the respective loading of these variables, compared with factor 1 and 2, they should be considered associated with adverse effects. Another situation occurs with heptachlor epoxid. This pesticide appears with higher loads in factor 3 than in factor 5. However in factor 3 the loads are negatively associated with positive loads of an adverse effect, so it should be in some way associated with adverse effects (revealed in factor 5).

From these factor analyses and from all the contaminants analyzed only the pesticides: γ–BHC, dieldrin and endolssulfan I, seem not to be causing adverse biological effects. Aldrin was not included in the FA due to all levels in the stations being above detection limit. Nevertheless FA consider each variable by themselves and it is important to keep in mind that biological effects are the result of interactions between geochemical features and forms and levels of the contaminants and moreover toxicity of a complex mixture is not necessarily the sum of their components toxicity.

Amphipod sediment bioassay showed, as expected, to be more related with the pesticides when comparded with metals.

The overall risk assessment for each management units, integrating the FA results (Fig. 11.3), the tabular matrix analysis and BPJ are shown in Table 11.3 and Fig. 11.4. Table 11.3 are listed the explanation of overall assessment and the contaminants of concern. For overall assessment the factors with low explicative variance were considered with care and always taking into account the raw data (see data in Table IX.1 in Annex IX).

From the FA it can be noticed that the metal's concentrations are associated together and with the organic load of the sediment (FF and TOM) and the benthos index (that was also based on sediment characteristics), and less associated with toxicity. Release of metals from estuarine sediments is determined primarily by sediment physico-chemical characteristics and secondarily by the level of resuspension energy (Turner *et al.,* 2002). Since in our study area their higher levels are associated with high organic loads and low levels of hydrodynamics (management units HO1, HO2, HO3, HO5 and HO6 – see Fig. 11.1 and Table 11.3) their retention is expected. Most of these areas where the heavy metals and metalloid are contaminants of concern correspond to areas in the North Channel near industries and urban sewages responsible for discharging these contaminants (see Table 11.3 and Fig. 11.4). The potential for metals release from sediments by bioturbation should be negligible on those areas due to the existent benthos community's characteristics. However, the meaning of interactions between sediment-bound metals and sediment-ingesting organism remains to be determined and further analysis of hazard identification, exposure, effects and risk characterization should be conducted for a correct ecological risk assessment (Chapman *et al.*, 2003). Bed sediment needs only to be moderately enriched in trace metals compared to suspended particulate matter to cause measurable addition of dissolved metal to the overlying water column (Martino *et al.,* 2002). Though according to Turner *et al.* (2002) trace metals in highly contaminated or organic-rich environments may be "squeezed out" of aqueous solution, suggesting that the effects might be a common characteristic of certain metals in the presence of a specific pool of organic ligands. These facts can explain the low association between the metals and the elutriate sediment bioassay.

As noticed by the FA interpretation, the different organochlorine pesticides have shown different behaviors and were found in different areas. From the fourteen pesticides analyzed the ones of highest concern in the study area are the DDT and its metabolites (in the management units HO3, HO5, MHO2, MHO5), and BHC isomers (in the management units HO1, HO2, HO6, LO2, LO3, MO1, MO2 and MO5 – Table 11.3). Also the pesticides heptachlor and heptachlor epoxid (LO3, HO5, HO6, MHO5), isodrin (HO5, MHO4), endolsulfan II (HO5, MO5) and endrin (HO5) were associated with adverse effects. For some of these pesticides there aren't available PEL values, what makes it difficult to determine their adverse effect evaluation. These pesticides are used as insectides usually in crops like rice and other cereal and vegetables (Laws, 1993). The use of most of these pesticides was banned in Portugal according to Portuguese law nº 348/88 (DR, 1988) and nº 660/88 (Portaria, 1988), due to their hazard and persistant characteristics. Isodrin was never homologated in Portugal. According to the European Directive nº 76/464/EEC (EEC, 1976) all these pesticides are considered dangerous substances (DDT, DDE, DDD, endrin, BHC's, isodrin in list I and endolsulfan II and heptachlor in List II), due to their toxicity, persistence and bioaccumulation, particularly for fish (Donze *et al.,* 1990).

The found concentrations of the pesticides, p,p'-DDE, p,p'-DDD and p,p' DDT were all below PEL levels but associations with biological adverse effects were found. Although these compounds were banned from most insecticide applications about 20 year ago, some authors showed that levels of DDT metabolites have increased in the environment (Anderson *et al.,* 1998). DDT can remain effective for up to twenty five years and the bio-accumulation of DDT can operate at different levels of the food chain (French, 1997). Organochlorine insecticides like DDT, were commonly and recently detected in sediment and aquatic biota in the USA even though their agriculture uses were discontinued during the 1970s (Nowell *et al.,* 1999). Earlier works conducted on the Sado estuary found levels of DDT and metabolites in sediments associated with industrial sources in the North Channel (e.g. Castro *et al.,* 1994).

Endolsulfan is a high toxic insecticide which application was not yet banned and which is still used in the rice fields in the Sado watershed, upstream the estuary. Toxicity tests conducted in the Sado River (Alcácer Channel) near the rice-field crops have shown that Endosulfan has high potential to cause adverse effects to the biota (Pereira, 2003).

Lindane (BHC isomer) is also used in rice-field crops in the Sado watershed (Pereira, 2003) and is a product largely used in Portuguese cultures (like in tomatos and corn, existent cultures near Sado), to clear off soils and stored products although it's commercialization is no longer allowed according to European Community law nº 2000/82/EC (EC, 2000).

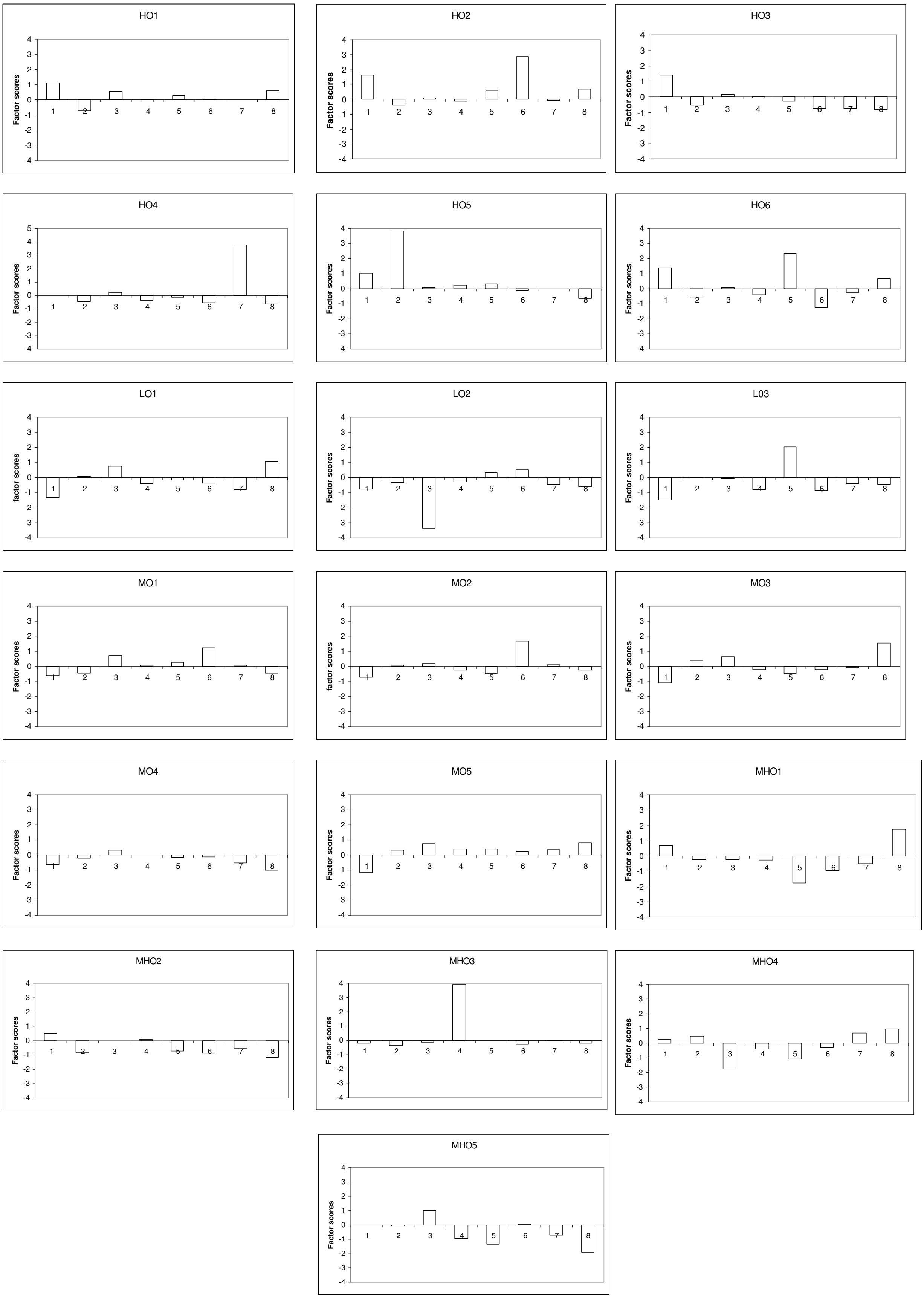


Figure 11.3 – Factor score estimated from FA for each management unit.

Table 11.3 – Tabular matrix with the SQT LOE for the management units. BOD-Biological Oxygen Demand; COD-Chemical Oxygen Demand; Nut.- Nutrients; SS-Total Suspended Solids; PAH-Polynuclear Aromatic Hydrocarbons; PCB-Polychlorinated Biphenyls; TBT-Tributyltin; FOG-Fat, Oil and grease; HC – Hydrocarbons.

Management units/Triad components	Chemistry		Toxicity		*In situ* alteration	Management type area	Main Driving Forces/Pressures	Pressure components (potential pollutants)	Overall risks assessment	Explanation/contamination of concern
	Metals and metaloids	Pesticides	Amphipod mortality	Urchin abn. larvae	Biotic Index					
HO1						Stable	• Urban (city of Setúbal) sewages and harbors	• BOD, COD, SS, Nut, FOG, HC, metals, acids, TBT, pathogens		• Potential significant adverse effects (benthos alteration) caused by heavy metals and metalloid and δ-BHC.
HO2						Stable	• Urban (city of Setúbal) and Industrial (Ferments, pyrites, power plant) sewages and harbors	• BOD, COD, SS, Nut, metals, PAH, FOG, HC, acids and bases, TBT pathogens		• High significant adverse effects (toxic and benthos alteration) caused by heavy metals and metalloid (Cd, Cu, and As exceed PEL levels) and δ–BHC. Higher concentration of α-BHC. Toxicity more associates with soluble compounds.
HO3						Stable	• Industrial (pulp and paper) sewages and harbor	• FOG, COD, BOD, acids and bases, PCB, metals, SS, cyanides, phenols, HC, TBT, pathogens		• Potential significant adverse effects (benthos alteration) caused by heavy metals and metalloid and p,p'DDD.
HO4						Stable	• Near areas of industrial and domestic sewages, sediment transport			• Unmeasured chemicals or conditions exist with the potential to cause degradation in the sediment (toxic and benthos alteration). Reduced sediment. Further investigations are needed.
HO5						Stable	• Industrial and domestic (shipyard and mine industry) sewages and run off, and harbors	• BOD, COD, acids and bases, PCBs, TBT, metals, PAHs, sulphides, FOG, HC, TBT pathogens		• High potential significant adverse effects (toxic and benthos alteration) caused by heavy metals and metalloids (Cd and Zn exceed PEL levels) and the pesticides Heptachlor, Isodrin, p,p'-DDE, p,p´-DDD, p,p´-DDT, endosulfan II and endrin.

Table 11.3 – Tabular matrix with the SQT LOE for the management units. BOD-Biological Oxygen Demand; COD-Chemical Oxygen Demand; Nut.- Nutrients; SS-Total Suspended Solids; PAH-Polynuclear Aromatic Hydrocarbons; PCB-Polychlorinated Biphenyls; TBT-Tributyltin; FOG-Fat, Oil and grease; HC – Hydrocarbons (cont.).

Management units/Triad components	Chemistry		Toxicity		*In situ* alteration	Management type area	Main Driving Forces/Pressures	Pressure components (potential pollutants)	Overall risks assessment	Explanation/contamination of concern
	Metals and metaloids	Pesticides	Amphipod mortality	Urchin abn. larvae	Biotic Index					
HO6	😐	🙂	🙂	🙂	🙁	Stable	• Non-point source pollution from Águas de Moura Channel (urban, fishing harbor rice-fields and aquaculture). It is inside the RNES	• Pesticides, Nut., BOD, COD, SS, pathogens	😐	• Potential significant adverse effects (benthos alteration) caused by heavy metals and metalloid (Cd exceed PEL levels), δ-BHC and Heptachlor epoxid.
LO1	🙂	🙂	🙂	🙂	🙂	Unstable	• Tourism, harbour	• FOG, HC, metals, acids, pathogens, TBT, COD	🙂	• This sediment does not present a risk. Reference area. Although with some pressure near the harbour this is a big area with high hydrodynamic with direct contact with the ocean, with no industrial pressure.
LO2	🙂	😐	🙁	🙂	😐	Unstable	• Non-point source pollution from Águas de Moura Channel (urban, fishing harbor, rice-fields and aquaculture). Near polluted areas (HO5). It is inside the RNES	• Pesticides, Nut., BOD, COD, SS, pathogens • Near pollutants of HO5	😐	• Potential significant adverse effects (toxic and benthos alteration). α-BHC or other unmeasured toxic chemicals are causing degradation. High levels of γ-BHC but not bioavailable. Further chemical investigations are needed. Due to surface sediment are less stable, analysis in sediment in depth should be conducted (Grapentine *et al*., 2002). Due to more hydrodynamics in this area toxicity could not be present in bottom water.
LO3	🙂	🙂	😐	🙂	😐	Unstable	• None direct but maybe from sediment transport		😐	• Potential significant adverse effects (toxic and benthos alteration) caused by δ-BHC, heptachlor epoxid or other unmeasured chemicals. Further chemical investigations are needed.

Table 11.3 – Tabular matrix with the SQT LOE for the management units. BOD-Biological Oxygen Demand; COD-Chemical Oxygen Demand; Nut.- Nutrients; SS-Total Suspended Solids; PAH-Polynuclear Aromatic Hydrocarbons; PCB-Polychlorinated Biphenyls; TBT-Tributyltin; FOG-Fat, Oil and grease; HC – Hydrocarbons (cont.).

Management units/Triad components	Chemistry		Toxicity		*In situ* alteration	Management type area	Main Driving Forces/Pressures	Pressure components (potential pollutants)	Overall risks assessment	Explanation/contamination of concern
	Metals and metaloids	Pesticides	Amphipod mortality	Urchin abn. larvae	Biotic Index					
MO1						Medium stable	• None direct but maybe contamination from sediment transport			• Potential significant adverse effects (toxic and benthos alteration) caused by α-BHC and δ-BHC or other unmeasured chemicals. Further chemical investigations are needed
MO2						Medium stable	• None direct but maybe from sediment transport			• Potential significant adverse effects (toxic and benthos alteration) caused by α-BHC or unmeasured chemicals. Further chemical measures investigations are needed.
MO3						Medium stable	• One domestic/industrial (pulp and paper) sewage. Near polluted areas (HO3 and MHO5)	• BOD, COD, SS, Nut., patogens, FOG, acids and bases, PCB, metals, cyanides, HC, phenols		• There is no immediate need for risk management evaluation, but further investigation is required. Due to surface sediment are less stable, and proximity of contamination sources analysis in sediment in depth should be conducted.
MO4						Medium stable	• Non-point source pollution (from Alcácer channel) and contamination from sediment transport. It is inside the RNES	• Pesticides, nutrients, BOD, COD, SS; pollutants transported from other areas		• Potential significant adverse effects (toxic) caused by unmeasured chemicals. Further chemical investigations are needed due to non-point pollution sources.
MO5						Medium stable	• Contamination from sediment transport. It is inside the RNES			• Potential significant adverse effects (toxic and benthos alteration) caused by δ-BHC and endolsulfan II.
MHO1						Medium stable	• Urban (city of Setúbal) sewages harbours	• BOD, COD, SS, Nut., FOG, HC, TBT, pathogens, acids		• Contaminants are not available. This sediment do not present a risk.

Table 11.3 – Tabular matrix with the SQT LOE for the management units. BOD-Biological Oxygen Demand; COD-Chemical Oxygen Demand; Nut.- Nutrients; SS-Total Suspended Solids; PAH-Polynuclear Aromatic Hydrocarbons; PCB-Polychlorinated Biphenyls; TBT-Tributyltin; FOG-Fat, Oil and grease; HC – Hydrocarbons (cont.).

Management units/Triad components	Chemistry		Toxicity		*In situ* alteration	Management type area	Main Driving Forces/Pressures	Pressure components (potential pollutants)	Overall risks assessment	Explanation/contamination of concern
	Metals and metaloids	Pesticides	Amphipod mortality	Urchin abn. larvae	Biotic Index					
MHO2	😐	😐	😐	🙂	😐	Medium stable	• Urban (city of Setúbal) domestic and Industrial (pesticides and fertilizers) sewages, and harbors	• BOD, COD, SS, Nut., Metals, DDT and other organo-chloride pestices, phenols, FOG, HC, acids, TBT, pathogens	😐	• Potential significant adverse effects (toxic and benthos alteration) caused by p,p´-DDT, p,p´-DDD or other unmeasured chemicals.
MHO3	😐	😐	😐	🙂	😐	Medium stable	• Tourism, military harbor, Non-point source pollution (rice-fields and agriculture) and contamination from sediment transport. It is inside the RNES	• Pesticides, nutrients, FOG, HC, metals, acids, pathogens, BOD, COD, TBT, SS	😐	• Potential significant adverse effects (toxic and benthos alteration) caused by unmeasured chemicals. Higher concentration of endolsulfan I and II, but maybe not bioavailable. Further chemical investigations are needed.
MHO4	😐	😐	😐	🙂	😐	Medium stable	• Non-point source pollution from Ag. de Moura and Alcácer Channels (urban, fishing harbors, rice-fields and aquaculture). It is inside the RNES	• Pesticides, nutrients, BOD, COD, SS, pathogens	😐	• Potential significant adverse effects (toxic and benthos alteration) caused by isodrin or other unmeasured chemicals. High levels of γ-BHC but not bioavailable.
MHO5	😐	😐	☹️	☹️	😐	Medium stable	• Industrial and domestic (fuel tanks, restaurant and shipyard) sewages, and harbor	• BOD, COD, HC, acids and bases, PCBs, TBT, metals, PAHs, FOG, HC, metals, SS, pathogens	☹️	• High significant adverse effects (toxic and benthos alteration) caused by heptachlor and p,p'-DDD or other unmeasured chemicals. Further chemical investigations are needed due to high levels of toxicity in both tests.

The areas where the pesticides with adverse effects were found are mainly on the North Channel or at the entrance of Águas de Moura (Table 11.3 and Fig. 11.4). Their presence and deposition can be not only related with the sediment transport from the rice-fields, the aquacultures and other agriculture crops but also from atmospheric deposition, non farm use or incidental release from chemical manufacturing plants (Nowell *et al.,* 1999) (like fertilize and pesticide industry located near management unit MHO2. Ferreira *et al.* (1990) and Castro *et al.* (1990) associated the presence of organochlorine residues in bivalves of the Sado estuary with run-off or accidental spills.

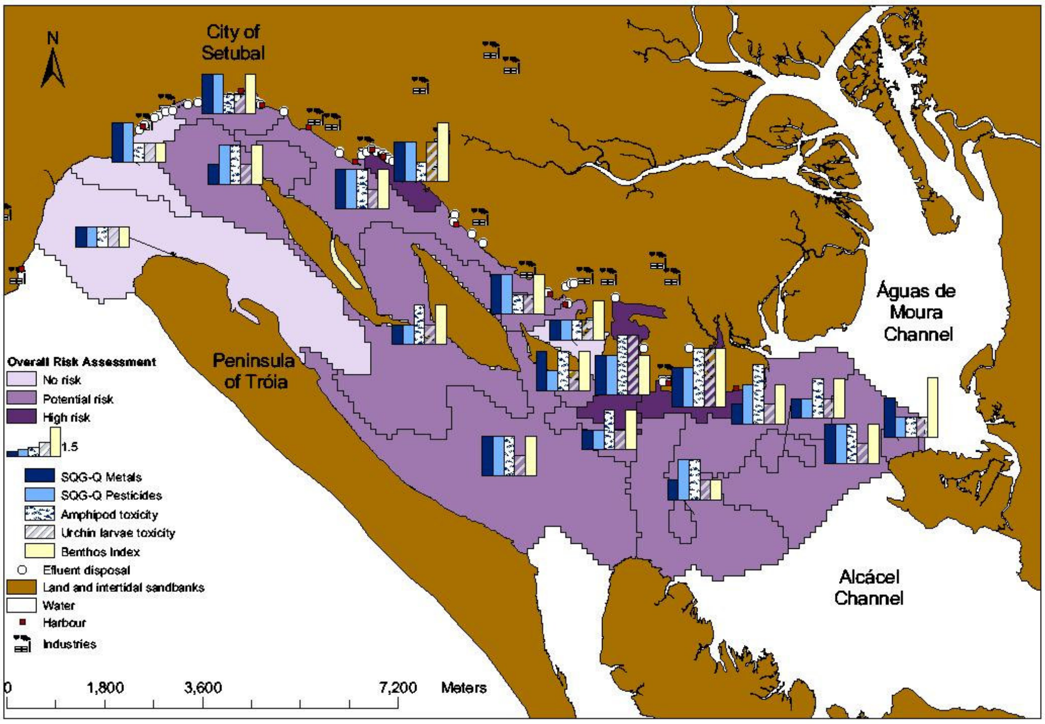


Figure 11.4 – Overall ecological risk assessment and LOE scores for each management area, according to Table 11.3. Industries adapted from Araujo *et al.,* (2002), effluents disposal from Correia and Florêncio (2002) and harbors from APSS, 2003.

In some management units classified with potential risk assessment, adverse biological effects were detected, however they were not directly related with the contaminants analyzed. Further chemical analysis should be conducted to measure PAH, PCB and TBT. These chemicals are discharged into the estuary by the existent anthropogenic sources (see Table 11.3) and several research works detected levels of concern of PCB (e.g. Castro *et al.,* 1994, Gil and Vale, 2001) and TBT (Quevauviller *et al.*, 1989b) in sediments and bivalves. Other pesticides, used by rice-field farmers in Sado watershed like Molinate, Propanil, MCPA and Clorphenvinphos, could also be measured. In particular chlorphenvinphos and Molinate have shown to be more associated with water toxicity in the river Sado (Pereira, 2003). Also other geochemical features such as the ammonia and sulfide contents in sediment, the contaminate-binding capacity of Acid Volatile Sulphide and total organic carbon can affect the toxicity results (Nipper, 2000).

Other LOE can be used like bioaccumulation or field toxicity (Nipper, 2000, Batley *et al.,* 2002). *In situ* toxicity is very complicated in estuaries mainly due to their high hydrodynamics. Measurement of contaminants in tissues of resident benthic fauna may provide evidence of bioavailability, and that the contaminants may be responsible for observed effects on the organisms. There is also the potential for these contaminants to biomagnify through the food chain producing adverse responses in higher trophic level organisms (Grapentine *et al.,* 2002). Nevertheless the quantification and interpretation of these LOE is still complicated and expensive. They could be measured only at particular places with chemicals of concern (Anderson *et al.,* 2001).

11.4 CONCLUSIONS

This paper provided tools for sediment quality assessment LOE, integrated with human activities and their Pressures in a BPJ, leading to future management recommendation. Providing managers with a defensible science-based recommendation in which they can be confident is crucial to moving to risk management decisions when factors beyond science have to be considered (Grapentine *et al.,* 2002). Even so, realistic and technically defensible applications of WOE need to recognize uncertainty and address the reality that, though uncertainty can be minimized, it can never be eliminated. Uncertainties in WOE sediment quality assessments can be due to several factors like sampling, transport and storage, sediment chemistry, ecotoxicology, benthic community structure, and data uncertainties and assurance or control quality (Batley *et al.,* 2002). These facts should be taken into account when the conclusions are drawn to the overall classification and definition of the contaminants of concern.

GIS and spatial analysis tools helped the overall sediment risk assessment integrating stressors and adverse effects in the ecosystem and visualizing it in an understanding way for decision –makers.

From the nineteen management units analyzed three don’t present any ecological risk (18.5 %

of the study area). The areas of more concern are HO2, MHO5 and HO5 (5.6 % of the study area) (Fig. 11.4). These areas of high or medium high organic load are located in the North Channel and suffer high human pressure mainly because of industrial activities. In particular the areas HO5 and MHO5 can also accumulate the contamination coming from Águas de Moura Channel, since particles coming from that channel can settle near Lisnave and Eurominas industries due to residual flow (hydrodynamics according to Neves, 1985). These areas have also low hydrodynamics, thus are associated with high levels of deposition. In addition they are just located near the limit of the Natural Reserve (see Fig. 11.1). In these areas the contaminants of concern, from the ones analyzed, are the heavy metals and metalloids, in particular Cd, Cu, Zn and As exceeded the PEL guidelines, and the pesticides BHC isomers, heptachlor, isodrin, DDT and metabolits, endosulfan II and endrin.

Due to methodological reasons the toxicity bioassays were conducted with sediments collected in the different campaigns of the chemical analysis. It was only possible to select the more representative stations of each management unit for the reduced toxicity campaign, after the chemical analysis was performed. The chemical sediment analysis of the second campaign, including metals and pesticides concentration when available should be compared with the data of the first campaign to confirm the association found between the bioassays results and the sediment chemistry.

Prior to final management recommendations an assessment of the physical stability of the sediment, and the likelihood of its disturbance by changes in flow regime or human activities should be performed (Grapentine *et al.,* 2002). A sediment transport model should be used to estimate which estuary management unit will suffer a *Pressure* and the resulting *State* and *Impact* (Painho *et al.,* 2002). In a near future maintenance dredging operations are to be conducted and changes in industrial processes and wastewater treatment improvements are expected. These *Pressures* will cause some change on the *State* and *Impact* of the present sediment quality turning this assessment even more important as a baseline and monitoring study.

Other important contaminants, PCB, PAH and TBT should be measured on the study area to complement the WOE approach, since unmeasured chemicals are probably causing adverse effects in some of the areas. In addition sub-lethal effects, DNA damage, metalotionines and lipoperoxidation levels will be evaluated in the survivors of the amphipod bioassay. In a short number of locations a chronic test with the fish *Sparus aurata* (14 days) was also conducted for evaluation of the same biomarkers. Biomarkers at organism level like DNA strand breakage have been proving to be very helpful for interpretation of toxicity testing within the multi-level assessment concept (Costa *et al.,* 2002).

All these data when available should help to improve the overall risk assessment of the management units and a better link with the estuary pressures. Nevertheless a burden-of-evidence approach must be balanced including more complete, with less uncertainty and less expensive analyses and fast an easy quality indicators.

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PART VI

GLOBAL CONCLUSIONS

CHAPTER 12 – GLOBAL CONCLUSIONS

CONCLUSIONS

Coastal zone management continues to be an emergent issue, where the development and experimentation of methods and tools are still fundamental. The geographic location of Portugal with more than half of its boundaries in connection with the ocean turns this matter even more important. Although some of the Portuguese estuaries already experience different CZM approaches not many efforts have been conducted to collect and manage data in an integrative way for a correct and clear approach to CZM. The Sado Estuary is a good example where such management is still needed.

The main objective of this thesis was to develop an estuary environmental management framework using the DPSIR Model (EMMSado), including data collection, data processing and data analysis. This framework was applied to the Sado Estuary (estuary bay) in Portugal. In this approach the human pressures for development (*Driving Forces* and *Pressures*) were evaluated in a preliminary stage and integrated with the Estuary *State* and *Impact*. These last categories were evaluated through sediment quality using a Weight of Evidence approach that also took into account human pressures. Environmental homogenous areas were delineated to be used as management units, the support for the estuarine quality assessment within EMMSado. To accomplish this main objective a multi-disciplinary work was put in practice.

As a global conclusion, from the nineteen management units delineated and analyzed three showed no ecological risk (18.5 % of the study area). The areas of more concern (5.6 % of the study area) are located in the North Channel and are under strong human pressure mainly due to industrial activities. These areas have also low hydrodynamics and are thus associated with high levels of deposition. In particular the areas near Lisnave and Eurominas industries can also accumulate the contamination coming from Águas de Moura Channel, since particles coming from that channel can settle down in that area due to residual flow (hydrodynamics according to Neves, 1985). In these areas the contaminants of concern, from those analyzed, are the heavy metals and metalloids (Cd, Cu, Zn and As exceeded the PEL guidelines) and the pesticides BHC isomers, heptachlor, isodrin, DDT and metabolits, endosulfan and endrin. In the remain management units (76 % of the study area) there is a moderate adverse ecological impact potential and in some of these areas no stress agents could be identified, emphasizing the need for further research, since unmeasured chemicals may be causing or contributing to these adverse effects. Special attention must be taken to the units with moderate adverse ecological impact potential located inside the natural reserve (HO6, MHO3, MHO4, MO4, MO5 and LO2). Non-point source pollution coming from agriculture and aquaculture activities also seem to contribute with important pollution load into the estuary entering from Águas de Moura Channel. This pressure is expressed in a moderate impact potential for ecological risk existent in the areas near the entrance of this Channel. Pressures may also came from Alcácer Channel although they were not quantified in this study.

The research of this study was organized in four main working lines, which are summarized in the next paragraphs. In each case a brief discussion will be presented, including the fulfillment of the specific objectives, the validation of the research assumptions and the enumeration of the limitations found during this work. In a final part the future research developments will be discussed.

Methodology definition and indicators selection for DPSIR

In the first phase global information about the Sado Estuary was acquired allowing to find out that this estuary is indeed subject to intensive human activities and pressures for development in spite of the fact that most of the estuary is classified as a natural reserve. Various specific and not integrated studies refer water, sediment and biota contamination and the existence of intensive fisheries activity. Along this work the quantification of the pressures and the estuarine quality assessment confirmed these statements, although high contamination levels were only found in restriced areas, usually associated with particular contamination sources or hydrodynamic conditions.

From the discussion of the existent different indicators framework, their primary objectives and target system, DPSIR has shown to be an appropriate model to collect, integrate and analyze data adequate for costal zone management.

An appropriate set of indicators for each DPSIR category was selected according to indicator's concept and criteria and data about the Sado estuary (Chapter 2). Different research and selected tools such as GIS, spatial analysis, including interpolation surfaces using geostatistics algorithms, GPS, multivariate statistics and Best Professional Judgment, were chosen to be integrated in the DPSIR. Along the work these tools have demonstrated to be very valuable to attain the objective of this study.

Delineation of management units

For the data collection and management units delineation, an extensive systematic unaligned sampling design was defined using prior information on the spatial variation in the estuarine sediments. A final grid of 750x500 was used to sample sediment parameters of general characterization (FF, TOM and Eh) (Chapter 3). This sampling was integrated into a GIS within a digitized Sado Estuary boundary after incorporating tidal information. The data of those parameters allowed the delineation of spatially contiguous areas, using different multivariate geostatistical tools according to three different methods (Chapter 4). After discarding the smallest areas, all the methods yielded 19 management units that demonstrated to be spatially contiguous and realistically represent the estuarine environment. Nevertheless it should be taken into account that the delineation of the units is dependent on the grid used for sampling and interpolation. In addition the approaches used for the management units for CZM delineation engaged complex computation.

Different and updated comparison approaches were used to evaluate and compare the maps similarities and to verify that using either single cell, hard or soft neighborhood comparison, their results are similar. The map similarity measurements used such as Kappa standard, Klocation, Khisto and assessment of budget components of agreement and disagreement in terms of quantity and location, demonstrate to be very useful and complementary to be applied in comparing maps just as they are for remote sensing, simulation modeling and land use change analysis (Chapter 5). This fact supports the choice of any of the methods as almost equivalent and thus of equal value. One of the methods (method 1) was chosen based on better agreement with the estuary behavior, assessment of contaminant sources and previous knowledge of the study area.

Social and economic pressures

The DPSIR indicators belonging to *Driving Forces* and *Pressures* categories were the first to be quantified. In a first stage the indicators were calculated only in Setúbal sub-watershed since the main human pressures of the estuary are located in this area. Sub-watershed units were defined as the terrestrial boundaries in which the indicators data were clipped. The choice of these terrestrial units was important for the data management and spatial evaluation of the estuary pressures within the DPSIR framework. This preliminary quantification was a difficult task to perform due to the lack of data. Much of the data, like the quantification of pollution loads were only possible to determine in a qualitative way. Although several plans and inventories were developed or are in development, most of them occurred in accordance with EU obligations and the availability of their data is very limited even for academic purposes (Chapter 6).

No substantial advantages were noticed in the division of *Driving forces* and *Pressures* categories, after their quantification and spatial representation. The *Driving Forces* indicators help to represent and list human activities (e.g. area occupied by rice-field) that are responsible for the *Pressures* (e.g. tonnes of pesticides used in rice-field). Also the indicators belonging to the *Driving Forces* category allow that the impact on sustainable development may be either positive or negative, as that is often the case with social, economic and institutional indicators. Nevertheless, the gain in precision does not compensate the use of *Driving Forces* category. An adaptation approach could be the single use of *Pressure* indicators though considering encompassing the human activities, processes and patterns that impact on sustainable development.

Sediment quality assessment

State and *Impact* categories of the DPSIR model were only quantified in the sediments due to well-known sediment importance to diagnose the environmental quality of estuarine ecosystems. This was demonstrated along the sediment quality assessment.

An optimisation model was used to choose the most representative monitoring stations inside each management unit, to assess sediment metal contamination in a cost effective way. This optimisation procedure was based on the minimization of the estimation error variance of the interpolation method used for management units delineation (indicator kriging). The model results indicated a design of 60 stations as optimal but 17 additional stations were added according to expert judgment since some of the management units wouldn't be sampled in the first optimal scheme solution. The sampling network thus chosen was statistically well justified and considered very important for an accurate evaluation for a baseline monitoring. But the main limitation of the optimisation procedure used was the fact that the management units were not considered as areas overlaid in the sampling points (Chapter 7).

Interpolation surfaces, GIS functionality and indices were used for the evaluation of estuarine sediment metal contamination. The use of these tools can make these evaluations less expensive and more understandable for the decision maker. The critical analysis of the different indices used and developed, alert for the need of an improvement in the methods standardization to allow a better comparability between indices and the simultaneous use of complementary indices.

The metal's concentrations measured in several locations in each homogeneous area (exception for five areas where only one location was measured) pointed out some variation within each management area. The large area at the South Channel (MHO3) showed the largest variability among stations and also the two stations of the small unit near pulp and paper industry (HO3) (Chapter 8).

A benthos index was developed to characterize the benthos habitat. This benthic biotope index predicts the occurrence of macrobenthic communities, from physical and chemical variables and using benthic data that was previously analyzed by other authors. The index has proved to be a valid tool to assess the spatial pattern of benthos habitat in a less expensive and more understandable way. Nevertheless, a limitation of the evaluation of this essential component for sediment quality assessment, (considering possible *in situ* alterations), was the lack of update data to validate the index (Chapter 9).

A network of 30 stations, obtained by means of an optimization procedure using the metal contamination data, was created o be used in the future as a long-term monitoring program. Although this monitoring campaign may not catch all the variability in each management unit it has a reasonable cost-benefit relation cost and technical benefit and assure that all the areas are sampled, including the stations with higher variability and contamination. A monitoring program that grabs all the variability would be too expensive and inappropriate for a management purpose (Chapter 10).

It was only possible to evaluate the organochlorine pesticide and the toxicity in one single location per management unit (19 locations from the 30 stations network) due to budget constraints. Nevertheless these chosen locations should characterize the worst scenario. Due to methodological reasons the toxicity bioassays were conducted in sediments collected in a second campaign at a different time of the chemical analysis. In fact the selection of the more representative stations of each management unit for the reduced toxicity campaign was possible, only after the analysis of chemical data. Also, it was not possible to have data available in time about the contamination assessment of the sediment samples collected for the toxicity bioassays (Chapter 11).

For the assessment of sediment quality indices were integrated with multivariate statistics and Best Professional Judgment. The approach used for the sediment quality assessment, a Weigh of Evidence approach using the Sediment Quality Triad, revealed to be very useful. In this approach overall ecological risk could be assessed with confidence. Once more GIS and spatial analysis tools helped the overall sediment risk assessment integrating stressors and adverse effects in the ecosystem and visualizing it in an understandable way for decision–makers. Nevertheless, the more realistic and technically defensible application of WOE still contains uncertainty that can never be eliminated. This fact should always be taken into account in the overall classification and definition of the pollutants of concern and associated human pressures.

As a final conclusion statement the management framework presented here, including all the methodological tools may be applied to other estuarine ecosystems, which will also allow a comparison between estuarine ecosystems in other parts of the globe.

Future research

A reduction of the number of management units can be accomplished using hard classification, yielding a model of estuary management that is easier to manage and less expensive to monitor. Despite of this, special care must be taken in this reduction since variation was found within each management units. A fine-tuning of the definition of the units should be conducted according to the type and level of the identified disturbances, taking into account that the management units where delineated to be integrated in a CZM approach where the scope is to find global trends and not the small scale variability. In addition other more automatic methods, fast and simple for sediment management units delineation can be developed and their robustness evaluated by comparison with those developed in this work.

The quantification, as precise as possible, of the complete set of the *Driving force* and *Pressure* indicators should be conducted not only in the Setúbal sub-watershed but also in the others sub-watershed in the neighborhood of the estuary. This will allow the overall assessment of the estuary pressures for development.

In October 2003 sediments from each type of benthic biotopes were sampled, for a better validation of the developed benthos index. Macrofauna will be identified down to species level and the benthic biotopes will be classified according to Rodrigues and Quintino, (1993).

The chemical analysis of the sediment of the second campaign, when it becomes available should be compared with the data of the first campaign to confirm the association found between the bioassays results and the sediment chemistry. Other important contaminants such as, PCB, PAH and TBT should be measured on the study area to complement the WOE approach, since unmeasured chemicals are probably causing adverse effects in some of the areas. In addition, sub-lethal effects, DNA damage, metallothioneins and lipoperoxidation levels will be evaluated in the survivors of the amphipod bioassay. In a short number of locations a chronic test with the fish *Sparus aurata* (14 days) was also conducted for evaluation of the same biomarkers. Biomarkers at organism level like DNA strand breakage have been proved to be very helpful for interpretation of toxicity testing within the multi-level assessment concept (Costa *et al*., 2002).

Improvements in in situ alteration and toxicity lines of evidence can also be conducted. Acording to DelValls *et al.* (2004) the better way to evaluate the benthic community structure is to meausure the contaminants in organism's tissue (bioaccumulation) and the use of biomarkers and evaluation of histopathological lesions in benthic organisms. Also according to that author specif designed tests should be conducted using truly estuarine species under correct environmental conditions to assess sediment toxicity in estuaries. Field toxicity bioassyas could be used using caging animals in the area of study to measure biomarkers, bioavailability (chemical residues), histopathology and/or even mortality (Martins-Días *et al.*, 2004).

Sediment Quality Guidelines should be constantly improved due to their advantages to protect human health and the environment and to allow the improvement of ecological risk guidelines at worldwide level. Improvements in the SQG to take into account grain size effects should also be made due to the well-known high degree of heterogeneity and variability existent in estuarine sediments. The complete data of Sediment Quality Triad when available can be used to converge on appropriate SQG for the Sado Estuary using the WOE approach. These site-specific guidelines should be published, to allow integration and adjustments with the already existent guidelines. Sediment assessment frameworks for different management purposes should be based on site-specific information generated to evaluate the predictive ability of SQG at a site of interest (Wenning and Ingersoll, 2002). However the use of Sediment Quality Values or Guidelines as a single Line of Evidence for sediment quality assessment required for decision-making, is generally inappropriate because they are based on limited toxicity data that considered only some exposure routes. A predictive ability of the benthic bioeffects ranges from multiple-contaminant exposure, based on SQG-Quotients can be developed for the Sado estuary as already developed by other authors in other ecosystems (Hyland *et al.,* 1999). In the long-term monitoring program the SQG-Quotients adjusted for the Sado Estuary can be set as a first screening tool and only for areas of concern should a combined WOE be used according to a tiered sediment assessment framework as defined by (Chapman *et al.,* 2002). Another sediment guidelines can be validated to classify the risk associated with a specific area, including the human health risk and the determination of Tissue Quality Guidelines (TQV). These TQV can be calculated using histopathological lesions in organisms where the toxicity tests were conducted and chemical concentrations in their tissues (Riba *et al., in press*).

A sediment transport model, already developed for the Sado estuary by other authors, should be used to estimate which estuary management unit will suffer a *Pressure* and the resulting *State* and *Impact* as already stressed in the work of Painho *et al.* (2002) (see Aneex II). Through the EMMSado link with the ecological and hydrodynamic model this framework will become a powerful management tool with *State* and *Impact* assessment and *Responses* actions forecast in one single tool.

When all the data of *Driving forces*, *Pressures, State* and *Impact* indicators becomes available and assessed, a Weigh of Evidence can be conducted using structured process for collecting and distilling knowledge from a group of experts by means of a series of questionnaires interspersed with controlled opinion feedback, like the Delphi method does (Linstone and Turoff, 2002) or using consensus ranking (Burton *et al.*, 2002).

The *State* and *Impact* categories were only evaluated in the sediment, but the other indicators listed in Chapter 2 should also be evaluated and quantified like the fisheries stock evaluation, effects on the quality of the organisms used in human diet, coastal line evolution, among other. In particular the coastal line already digitized in the present work allows an accurate study of the shoreline evolution and changes owing to tidal information.

The data and management units characterization was developed using only one time series. It was not the aim of this work to evaluate seasonal, annual or any temporal differences. The *State* and *Impact* data presented in this work can be set as a baseline situation for future long-term monitoring campaigns. The indicators selected should be used to evaluate long-term monitoring anthropogenic changes in the ecosystems. With this type of survey a baseline of data can be produced and the performance of those indicators can be tracked down through time. With this type of information resource managers can make informed decisions on how to best protect environmental resources (Macauley *et al.,* 2002). This baseline data should be applied not only for comparing differences between time periods but also with other Portuguese, European or worldwide estuaries.

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ANNEX I – ENVIRONMENTAL INDICATOR FRAMEWORKS TO DESIGN AND ASSESS ENVIRONMENTAL MONITORING PROGRAMS

ENVIRONMENTAL INDICATOR FRAMEWORKS TO DESIGN AND ASSESS ENVIRONMENTAL MONITORING PROGRAMS

Ramos, T. B., Caeiro, S., Melo, J. J. (2004)

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ABSTRACT

Monitoring is a fundamental issue within Environmental Impact Assessment (EIA). It is important both to assess adherence to standards and to support management options. Worldwide concern about resource optimization and better environmental monitoring programs has led to increasing efforts to use new methodological approaches. The use of indicators assures that a monitoring program addresses only the key variables associated with significant environmental impacts and also improves monitoring communication and reporting processes. The main goal of this work is the development of a conceptual framework to design and assess an environmental post-decision monitoring program under EIA procedures – INDICAMP. Another aim of this paper is to discuss how current indicator frameworks can be used to design and evaluate the performance of environmental monitoring programs in projects. A coastal infrastructure case study is presented and the usefulness of this methodology is demonstrated.

KEY WORDS: Environmental indicators, monitoring programs, design, performance evaluation, projects, EIA follow-up.

I.1. INTRODUCTION

In recent decades a great deal of experience has been built up at an international level in the field of EIA. However, emphasis has been mainly focused on pre-decision analysis, with little understanding as to whether environmental impact assessment achieved its goals for environmental protection and management (Morrison-Saunders *et al.,* 2001). EIA follow-up is concerned primarily with the post-decision stage, including activities such as monitoring and auditing, e.g. post-evaluation or post-decision analysis, and so it is essential to keep track of the real effects projects have on the environment. In addition, this follow-up is an incentive for improving the environmental management quality of projects as well as permitting and enforcement processes (Glasson *et al.*, 1999). Despite being well defined, the implementation of EIA follow-up is rather difficult to measure owing to inadequate techniques, deficiencies in the Environmental Impact Statement (EIS) and resource limitations (Morrison-Saunders, 1996, Arts *et al*. 2000, Arts *et al*. 2001). It also receives less attention in the literature than other aspects of the EIA process (Noble, 2000, Morrison-Saunders *et al.,* 2001).

Among all the EIA follow-up activities, monitoring is the most continuous. It provides the data for the other activities and allows project and environmental performance objectives to be attained. Arts and Nooteboom (1999) define monitoring as a program of repetitive observation, measurement and recording of environmental variables and operational parameters over a period of time for a defined purpose. Monitoring can be considered at a pre- or post-decision project stage. *Pre-monitoring*, also called *baseline monitoring*, measures the initial state prior to implementation of a proposal. *Post-decision monitoring*, includes monitoring activities undertaken to determine the impacts or changes to the environment caused by the proposal once it has been implemented (environmental effects monitoring). It equally covers activities undertaken to ensure that environmental components are not altered by human activity beyond a specific standard or regulation level (*compliance monitoring*) (Lohani *et al.,* 1997, Morrison-Saunders and Bailey, 2001). Another type of monitoring is *area-wide monitoring*, which measures the general state of the environment in an area (Arts *et al.,* 2001). Tomlinson and Atkinson (1987) also discussed extensively terminology related to environmental auditing and monitoring. One additional new monitoring level could be the *meta-level monitoring*, which evaluate the performance of a monitoring program. Latter on this paper this new approach is explained in more detail.

Follow-up not only provides information about the consequences of an activity as they occur but also gives the responsible parties (proponent and/or competent authorities) the opportunity to take appropriate measures to mitigate or prevent negative effects on the environment. EIA follow-up can be seen then as the missing link between EIA and project implementation (Arts *et al.,* 2000), giving essential feedback to improve the EIA process. However such follow-up in post-consent decision stages is performed in only a minority of cases (Arts *et al.,* 2001) and in many countries is probably the weakest step in the process (Glasson *et al.,* 1999). Morrison-Saunders and Bailey (1999) found some weaknesses in the scope and rigor of environmental monitoring programs in Australian cases studies where these programs have not been able to determine whether or not potential environmental impacts have occurred. Sample contamination, lack of training and expertise in sampling and data analysis, uncertainty over the scientific integrity of monitoring programs, unsuitable spatial and temporal distribution of sampling sites, and no replication of sampling can be the reasons for inadequate monitoring (Morrison-Saunders and Bailey, 2001).

Discretionary measures are not enough and monitoring needs to be more fully integrated into EIA procedures on a mandatory basis (Glasson *et al.,* 1999). Also in places where EIA follow-up is a discretionary or even mandatory requirement (e.g. Canada, California, Hong Kong, Western Australia, the Netherlands and Portugal), it has proved difficult to put post-EIA monitoring and evaluation into practice (Arts *et al.* 2000, Morrison-Saunders and Bailey 2001). In Portugal, Decree-Law 69/2000 and Ministerial Order 330/2001 regulate ongoing EIA, where EIA follow-up is required. As already described by Jesus (2000), according to this law monitoring programs must be established in the EIS and proponents should periodically submit monitoring reports to the EIA authority. The EIA authority may impose project or management adjustments and/or additional mitigation in the case of unpredicted negative impacts. Additionally, EIA authorities can perform audits to verify compliance of project construction, operation or decommissioning with the original EIA decision and also to verify the accuracy of monitoring programs.

An important reason for the less than satisfactory performance of environmental monitoring programs may be that they were set up in the past for a variety of purposes, most of them derived from local or national priorities. They have not been designed to contribute to a synthesis of information or to evaluate project impacts, or analyze the complex cross-linkages between environmental quality aspects, impacts and socio-economic driving forces (UNEP/RIVM, 1994). Also, environmental monitoring initially focused on obvious, discrete sources of stress such as chemical emissions. It soon became evident that remote and combined stressors, while difficult to measure, also significantly alter environmental conditions. Consequently monitoring efforts began to examine ecological receptors, since they expressed the effects of multiple and sometimes unknown stressors (Jackson *et al.,* 2000). Because of the content of most stressor-response relationships, it is impossible to completely characterize all the variables, so a selected set of measurements should be made to reflect the most critical components. Such measurements, or indicators, should be included in monitoring programs to estimate trend, stressor source and magnitude of effects and lead to thresholds for management or restoration action (Fisher *et al.,* 2001).

One of the main aims of environmental indicators is to communicate information about the environment and human activities. To highlight emerging significant environmental impacts during monitoring programs, indicators can be especially useful. In an EIA process, public communication and participation, particularly monitoring data reporting, is a priority issue for strengthening post-decision monitoring that could be assured and improved by the use of indicators.

Impacts of projects need to be monitored on a regular basis during the entire project life cycle. Such monitoring should provide an account of EIA performance, regulatory compliance, mitigation performance evaluation, validation of impact-prediction techniques, verification of residual effects and linkages into contractual permitting, licenses and other management systems (Canter, 1996, Morrison-Saunders *et al.,* 2001). Targeting these factors and their lack of effectiveness in the monitoring programs is then crucial to evaluate their performance. This performance evaluation, though very important, is almost never done.

The measuring of management success is now required by the United States Government Performance and Results Act of 1993, whereby agencies must develop program performance reports based on indicators and goals (Jackson *et al.,* 2000). Along with this present priority at US level, a global trend in environmental performance evaluation is emerging, applicable to all types of organizations and specially supported by the ISO 14031 standard. This approach could be extrapolated to performance evaluation for project or plan monitoring programs.

The main goal of this paper is the development of a conceptual indicator framework to design and assess post-decision monitoring programs under EIA – INDICAMP. This framework aims to contribute to an improvement in monitoring program effectiveness, particularly in impact prediction accuracy and project environmental management activities. For that purpose there is a discussion of current indicator frameworks developed by various authors and of how they can be used to design and assess environmental monitoring programs for projects. The INDICAMP framework also includes indicators of monitoring performance, metal-level monitoring, aimed at evaluation of the quality and effectiveness of the monitoring program. This framework is applied to a coastal infrastructure case study in Portugal, submitted to an environmental assessment in order to test its applicability, advantages and drawbacks.

I.2. CONCEPTUAL FRAMEWORKS FOR INDICATORS

Despite the current importance of environmental indicators at international level, their development and use is not a very recent issue since the first important references date from the seventies, e.g. Thomas (1972); Inhaber (1976) and Ott (1978). More recently, several studies have presented guidance on developing environmental indicators, discussing indicator properties and criteria for their selection, e.g. Vos *et al*. (1985); Jeffrey and Madden (1991), Braat (1991), Gouzee *et al*. (1995), UNEP/RIVM (1994), Ramos (1996), Melo *et al.* (1996), HMSO (1996), FSU/USEPA (1996a, 1996b, 1996c, 1996d, 2001); Ramos *et al.* (1998) and EEA (1996, 1998, 1999).

Despite all these studies, the terminology used in the area of environmental indicators is still rather confusing and is not well established. The term "indicator" is sometimes used rather loosely to include almost any sort of quantitative information (UNEP/RIVM, 1994). Equally, statistics are often called indicators without being carefully selected or reworked. Various initiatives try to clarify environmental indicator typology. In particular, the EEA (1999) attempts to help policy-makers understand the meaning of the information in indicator reports and helps to define common standards for future indicator reports by the European Environment Agency. In order to keep the concept of an environmental indicator clear in this paper, the definitions of Ott (1978) and Jackson *et al*. (2000) were adopted: a sign that conveys a complex message, potentially resulting from numerous factors in a simplified and useful manner. An environmental indicator is derived from a single variable to reflect some environmental attribute.

Canter (1996) refers to the usefulness of using environmental indexes and indicators in terms of EIS, especially for baseline monitoring or monitoring studies in general, or also for prediction and impact assessment with regard to environmental components. The use of indicators is already being used in pre- and post-decision monitoring, as suggested in the works of Lohani *et al.* (1997) and Glasson *et al*. (1999). However, many of the studies under-explore the use of indicators in post-decision monitoring programs.

To assure that indicators serve the purpose for which they are intended and control the way they are specifically selected and developed, it is important to organize them in a consistent framework. Table I.1 presents an overview of indicator frameworks based on the chronological frameworks evolution and covers: i) the scale they were ideally built for, ii) their primary objective, iii) the target system that they focus on, and iv) comments and/or drawbacks. Despite the large variety of frameworks developed, many of them are quite similar in their methodological approaches and are mostly adaptations of the Pressure-State-Response (PSR) model, based on causality chains. Also, a variety of terms are used in different ways to cover similar categories, an issue which is broadly discussed by USEPA (1995) for some of the frameworks presented in Table I.1. On the other hand, the same item can appear in different places in a single/the same framework, depending on which target system we are focusing on.

Table I.1 shows how the frameworks evolve mostly from the assessment of the environmental systems to, more recently, the environmental performance of organizations/sectors or project evaluation. Many of them take into account not only the environment, but also the society and economy, attempting to measure sustainability. Generally, indicator frameworks were not developed with the purposes of EIA application, since the relation between them and EIA, post-decision in particular, is mostly non existent. Nevertheless, some EIS use indicators and/or indices, especially in pre-decision stage although without any formal framework.

The classification of the different types of monitoring indicators and the causality chains used by many of the indicator frameworks can be relevant to fulfill the purposes of EIA follow-up. According to Arts *et al.* (2001), one of the EIA follow-up objectives is to enhance scientific knowledge about environmental systems, particularly the cause-effect relationships. While cause-effect relationships are difficult to establish, environmental decision-making commonly relies on assumptions about such linkages in order to determine appropriate management responses. Thus, models and analyses, which show relationships among variables generally, have the most meaning for environmental decision-makers (USEPA, 1995). Nevertheless, special attention must be paid when using these causality chains not to suggest linear relations, to avoid obscuring the more complex relationships in the environment and the interactions among sub-systems.

Equally, monitoring should employ short feedback cycles and should quickly yield results in order to make the aim of EIA follow-up clear (Arts *et al.,* 2000). The use of these indicator frameworks can help to give these quick responses and improve the existing lack of efficiency in monitoring follow-up and also help to evaluate the performance of the monitoring programs (metal-level monitoring).

Table I.1 – The conceptual frameworks of environmental indicators.

Author/Year	Framework Name: Indicator Categories	Scale*	[a] Primary objective(s) and [b] target system	Comments /Drawbacks
Friend and Rapport (1979)	STRESS: Stress – Response	N	[a] Environmental statistics; resource accounting; [b] Environmental.	Physical basis for comprehensive environmental/resource accounts, which could be linked to the UN System of National Accounts. Unrealistic; tried to make one-to-one linkages among particular stresses, environmental changes and responses (USEPA 1995). "*Stress*" categories include natural as well as human influences and "*responses*" stands on ecosystems responses (UNEP/RIVM, 1994).
UN (1984)	FDES – Framework for the Development of Environmental Statistics: Statistical "Topics"	N	[a] Environmental statistics; resource accounting; [b] Environmental.	Expands and modifies STRESS framework. States the relation between information categories, representing a sequence of action and reaction to "environmental components" or "media" (Bartelmus, 1994). Incorporates social, demographic and economic statistics that are related to environmental concerns. Information categories are based on the recognition that environmental problems are the results of human activities and natural events.
Hamilton (1991)	PEP – Population Economy Process: Stocks – Processes – Interactions	N	[a] Environmental statistics; [b]Environmental/social/economic	Shows the interaction between society, economics and the environment. Considers the world divided into the three indicator categories and attempts to identify the *interaction* represented by flows between these categories. Each is characterized by its *stocks* (or *states*), *processes* (or activities) (Cardno, 2000; Hodge, 1997). Has an explicit link with the UN System of National Accounts (USEPA, 1995).
OECD (1993)	PSR: Pressure – State – Response	N	[a] Countries' environmental performance reviews; [b] Environmental.	Adapted from STRESS model. Based on a concept of causality: human activities exert pressures on the environment. These *pressures* modify the *state* of the environment, including socio-economic related aspects. Undesirable impacts lead to a *response* from society that results in the formulation of an environmental policy. According to Kelly (1998), fails to capture information about the structure and behavior of the systems in which decisions are made and fails to capture the complexity of the relationships in complex systems.
Barber (1994)	EMAP indicator framework: Condition – Stressor	L to N	[a] Estimate of the condition of the nation's ecological resources; [b] Environmental.	Environmental Monitoring and Assessment Program (EMAP) framework includes linkage of indicators to ecological and human values. *Conditions* and *stressors* are strictly related with *state* and *pressures* from PSR model.
Bartelmus (1994)	FISD – Framework for Indicators of Sustainable Development: Statistical "Topics"	N	[a] Sustainable development statistics; [b] Environmental/social/economic/institutional.	FISD are mostly FDES-based "*statistical topics*". Links concerns and programs of Agenda 21 with data framework of FDES, in order to obtain a framework which combines sustainable development concerns with environmental and related socio-economic data.
UNEP/RIVM (1994); RIVM (1995) Adopted by the European Environment Agency	DPSIR: Driving Forces – Pressures – State – Impacts – Responses	L to C	[a] Environmental assessment; [b] Environmental – includes human health, ecosystems and materials.	Similar to PSR framework, but with two more categories: i) *driving forces*, referring to the "needs" of individuals and institutions that lead to activities that exert *pressures* on the environment. The "intensity" of the *pressure* depends on the nature and extent of the *driving forces* and also on other factors which shape human interaction with ecological systems. ii) *impacts*: on ecosystems and human well being due to *state* modifications. The policy *responses* lead to changes in the DPSIR chain. *Greeuw et al. (2001)*state that a key issue is that the same item can appear in different places in the framework, depending upon which target we are focusing on.
USEPA (1995)	PSR/E: Pressure – State – Response – Effects	L to N	[a] To produce an integrated system of environmental information; [b] Environmental – includes human health and welfare.	Adapted from PSR framework and a derivative category called "*effects*" is added, for attributed relationships between two or more *pressure*, *state*, and/or *response* indicators; Pressures of non-human origin are also included in the framework.

Table I.1 – The conceptual frameworks of environmental indicators (cont).

Author/Year	Framework Name: Indicator Categories	Scale[*]	[a] Primary objective(s) and [b] target system	Comments /Drawbacks
UN (1996); UN (2001)	DSR: Driving Force – State – Response	N	[a] To make indicators of sustainable development available to decision-makers at the national level; [b] Environmental/social/economic/institutional.	Adapted from PSR framework; *driving force* instead of *pressure* in order to encompass human activities, processes and patterns that impact on sustainable development; driving force allows that the impact on sustainable development may be both positive or negative, as is often the case with social and economic and institutional indicators; No causal relationships among the three types of indicator.
Dixon *et al*. (1996); Segnestam (1999)	Indicator framework: Input – output – outcome – impact	L to G	[a] To assess and evaluate the performance of World Bank projects in relation to environmental issues; [b] Project.	Is based on the project cycle itself and is related with PSR framework. *Input* indicators monitor project-specific resources provided; *output* indicators measure goods and services provided by the project; *outcome* indicators measure the immediate, or short-term, results of the project implementation; *impact* indicators monitor the long-term or more pervasive results of the project.
Azzone and Noci (1996)	Performance Indicators Integrated Framework Integrated Framework of Performance Indicators: State – Policy – EMS – Eco-balance	L	[a] To evaluate corporate environmental performance; [b] Organization – corporate.	Integrated framework of which the main aim is to support environmental performance indicators at company level. Corporate environmental policy is the basis of the framework. Starts with the identification of the key environment-related factors to be included in the company environmental report and also defines how environmental performance can be expressed and how distinct measures can be aggregated to achieve a more complex picture.
Rotmans and Vries (1997)	PSIR: Pressure – State – Impacts – Response	N to G	[a] Sustainability assessment; [b] Environmental/social/economic/institutional	Several authors present PSIR as one more variant of the PSR framework, adding the category '*impact*', that can be seen as a measure of change in *state*. In some ways this framework has many similarities with DPSIR.
Federal Environment Ministry (1997)	Corporate Environmental Indicators: Environmental Performance – Environmental Management – Environmental Condition	L to G	[a] To evaluate corporate environmental performance; [b] Organization – corporate.	Despite similarities with the ISO 14031 indicator framework, presents different indicator categories and subcategories.
US Interagency Working Group on Sustainable Development Indicators (1998)	SDI framework: Long Term Endowments and Liabilities – Processes – Current Results	N	[a] Developing an experimental set of sustainable development indicators as a first look for key US economic, environmental and social well-being factors; [b] Environmental/social/economic.	SDI framework builds on the PSR model, but it accommodates a range of processes (both positive and negative) related to economics, the environment and society. It divides the "*state*" category into two separate categories: "*Long Term Endowments and Liabilities*" and "*Current Results*". *Processes* include human activities, natural earth systems processes and social, cultural or political/decision-making processes, related with *driving forces*, *pressures* and *responses* categories.
Meadows (1998)	Framework for sustainable development indicators: Natural Capital – Built Capital and Human Capital – Human Capital and Social Capital – Well Being	L to G	[a] To evaluate sustainable development; [b] Environmental/social/economic.	Based on a "Daly triangle/pyramid", a diagram created by Daly (1973), which relates natural wealth to ultimate human purposes through technology, economics, politics and ethics.
Personne (1998)	PER Enterprise: Pressures – State – Responses	L to G	[a] Enterprise environmental performance evaluation; [b] Organization –enterprises.	Adapted from PSR framework to develop enterprise performance indicators.
ISO (1999)	ISO 14031: Environmental Performance Indicators (Operational Performance Indicators (OPIs) and Management Performance Indicators (MPIs)) – Environmental Condition Indicators (ECIs)	L to G	[a] To evaluate an organization's environmental performance; [b] Organization – private or public of any size or type.	Despite the different nomenclature used, the main concepts are strictly related to a general PSR approach. The main difference is that in this model the main target is an organization and not the environment. The ECIs are the same as the *state* category. The OPIs (similar to the *pressure* category) provide information about the environmental performance of the organization's operations. The MPIs (similar to the *response* category) provide information about management efforts to influence the environmental performance of the organization. This framework was specially designed for organizations but in practice could be extrapolated to other types of "entities", like a country or a project.

Table I.1 – The conceptual frameworks of environmental indicators (cont).

Author/Year	Framework Name: Indicator Categories	Scale*	[a] Primary objective(s) and [b] target system	Comments /Drawbacks
Chesapeake Bay Program/USEPA (1999)	Hierarchy of Indicators: Administrative (1. actions by federal or state regulatory agency; 2. responses of the regulatory community or society) – Environmental (3. changes in discharge of emission quantities; 4. changes in ambient conditions; 5. changes in uptake and/or assimilation; 6. changes in health, ecology of other effects)	L	[a] Environmental assessment; [b] Environmental – includes human health and ecosystem.	This framework is an indicator-driven planning process that successfully uses an extensive range of environmental indicators that focus actions on the improvement of the resource. Levels 1 and 2 correspond to *response* indicators, level 3 shows *pressure* indicators and levels 4, 5 and 6 are *state* and *impacts* indicators. To measure the quality of each indicator with respect to the strength of the type of data, they developed a six-point scale for rating indicators. This framework is used for the primary purpose of communicating the health of the Chesapeake Bay and its rivers to public audiences.
USEPA (1999)	Indicator framework of the environmental impact of transportation: Activities – Outcomes – Outputs	R, N	[a] Identifying environmental impact of transportation; [b] Sector – transport.	This framework is based on three main stages. Transportation related *Activities* – like infrastructure construction, travel, and maintenance – result in releases of pollutants or damage to habitats. These *outputs*, in turn, have human health and welfare Effects – *outcomes.* Although developed for transport, can be used for other sectors; method based on causality chain approaches, like PSR, DPSIR, PSR/E.
EEA (2000)	Sector-environmental integration indicators: Socio-economic performance of the sector – environmental performance of the sector – eco-efficiency performance of the sector – monitoring implementation of integration measures and policy effectiveness	R, N	[a] To provide a coherent system of integration indicators that ensures co-ordination between indicators; [b] Sector-policy sector.	*Socio-economic* indicators category will measure the development in the sector size and shape, and how it is determined. The category "*environmental performance of the sector*" is based on environmental *pressure*, *state* and *impact* indicators. The *eco-efficiency* category provides the relationship between economic and environmental performance. After sector integration strategy has been finalized and implemented, monitoring of implementation and success of the policy measures should follow integration *of measures and policy effectiveness* indicators. (Hertin *et al.,* 2001) state that this framework is too focused on the environmental dimension of sustainability with too little consideration being given to the social and economic dimensions.
Hyman and Leibowitz (2001)	JSEM Judgment-based Structural Equation Modeling	L	[a] Environmental assessment; [b] Environmental.	Uses the framework of the Structural Equation Model (SEM), which combines path analysis with measurements models, to formalize available information about potential indicators and to evaluate their potential adequacy for representing an endpoint. Uses expert judgment regarding the strengths and shapes of indicator endpoint relationships.
FSU/USEPA (2001)	CAPRM Model: Administrative – Environmental	R to N	[a] Environmental assessment; [b] Environmental.	Based on the Hierarchy of Indicators and on the PSR/E framework.
Hertin *et al,* (2001)	Enterprise policy integration indicators: Headline – Integration – Process	R to N	[a] To monitor the integration of environmental and sustainable development into enterprise policy; [b] Sector – enterprises – industry.	These indicator categories are concerned with economic, social, and environmental outcomes (*headline* indicators), with identifying significant overlaps between enterprise policy and sustainability (*integration* indicators), and with monitoring how enterprise policy processes take into account sustainability objectives (*process* indicators).
Berkhout *et al*, (2001)	MEPI indicator framework: Physical – Eco-efficiency – Impact	L, R, N	[a] To measure the environmental performance of industry; [b] Sector – industry.	Includes primarily quantitative indicators and is focused on data generated by firms and production sites. *Physical* indicators measure mass, energy and waste flows through manufacturing processes; *eco-efficiency* indicators link physical data to data on business performance; *impact* indicators link physical data on inputs and emissions to measurable impacts on human population and the environment. Not developed for use by non-professional and lay audiences. Business and environmental analysts, policy makers, and business managers are potential user groups.
Marsanich (n.d.)	FEEM EMAS environmental indicators: Environmental Management – Environmental Absolute – Environmental Performance – Potential Effects – Environmental Effects	L to N	[a] To communicate companies' environmental performance in EMAS environmental statements; [b] Organization.	Based on ISO 14031 indicator framework. It established a modified classification of environmental indicators with modified and new categories and greater emphasis on environmental effect indicators.

*Spatial scale: L – local; R – regional; N – national; C – continental; G – global

I.3. DEVELOPMENT OF THE CONCEPTUAL FRAMEWORK

In the first stage of an EIA process, i.e., during project planning and design, it is fundamental to measure the initial state prior to implementation of the project – pre-decision monitoring. Only when the project is being implemented can we undertake monitoring activities to evaluate the impacts on the environment caused by the project (post-decision monitoring). These impacts can be evaluated when compared with the pre-decision monitoring data. (Fig. I.1). The main components of post-decision monitoring programs and its related goals can be described with indicators (see bottom text boxes on Fig. I.1). Three components are of particular importance, as underlined in Fig. I.1: select and develop monitoring indicators; define methods of communicating and reporting results outputs; define reviewing procedures and indicators of monitoring performance evaluation.

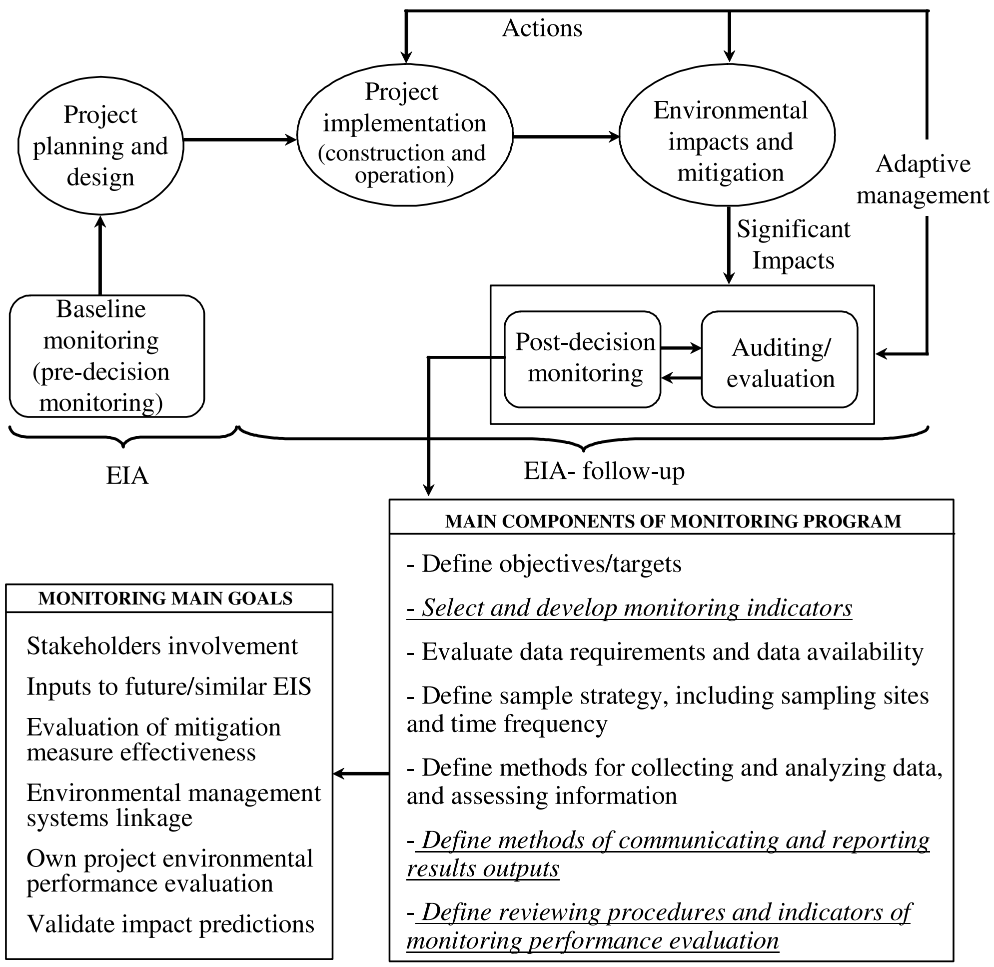

Figure I.1 – Environmental post-decision monitoring program: main components derived from an EIA with an indicator approach.

The post-decision stage should be included in a flexible approach to EIA (adaptive management activities), to enable and actively encourage ongoing refinements and improvements to management and monitoring programs (Morrison-Saunders, 1996; Noble, 2000). Additionally, the post-decision monitoring program should be based on a series of components, essential to ensure its effectiveness and fulfillment of its goals. In the approach here developed one of the principal components of monitoring programs is the selection and development of the monitoring indicators.

Based on a rearrangement of the frameworks PSR/E, DPSIR and ISO 14031 presented earlier, a new environmental indicator framework to design and assess post-decision monitoring programs – INDICAMP – was then developed (Fig. I.2). This framework tries to incorporate a systems analysis approach, designing the main cause-effect relationships between the different categories of monitoring indicators (*pressures, state, effects and responses*). It also includes *monitoring performance* indicators category to assess the effectiveness of the monitoring program itself. This kind of tool could help in applying the comprehensive or targeted environmental monitoring concept used by Canter (1996), (i.e. the establishment of cause-effect relationships), as well as in impact management and related corrective action.

This model shows how each project activity produces *pressures* on the environment, which then modifies the *state* of the environment. The variation in *state* then implies *effects* or *impacts* on human health and ecosystem receptors, causing project proponent and society to *respond* with various management and policy measures, such as internal procedures, information, regulations and taxes (see the dashed lines in Fig. I.2). The particular features of each of these categories follow the general methodology developed by RIVM (Netherlands Institute of Public Health and the Environment), (1995). Within EIA, e*ffects* indicators are particularly important since *state* indicators sometimes do not evaluate their impact on the environment by themselves. As an example, an increase in the heavy metal content of an environmental component due to project operation does not necessarily mean a pollution effect on organisms. *Effects* in some way concern relationships between two or more indicators within any of the *pressures*, *state* and *responses* categories.

The framework also shows that the performance of the monitoring program can be evaluated at one main stage – meta-level monitoring. At this level, *monitoring performance* indicators category represents the effort to conduct and implement the program, measuring also program effectiveness. The *monitoring performance* indicators will allow the following (see the dashed lines in Fig. I.2):

i) how appropriate the environmental and social-economic monitoring indicators are (*state*, *pressures*, *effects* and *responses* categories), leading to a review of and improvement in these components.

ii) evaluation of overall monitoring activities and results, including the environmental impact of the sampling process itself, to measure how well the monitoring program is going.

iii) evaluation of project environmental performance and impact mitigation action.

This category of *monitoring performance* indicators may be viewed as a *response* and *management* category (see ISO 14031 indicator framework in Table I.1), linked with the organization responsible for the monitoring program, where the target is the post-decision monitoring system. This should be distinguished from *response*-type indicators, which describe the responses of the project proponent/society as a whole and in which the targets are the environmental, social and economic systems.

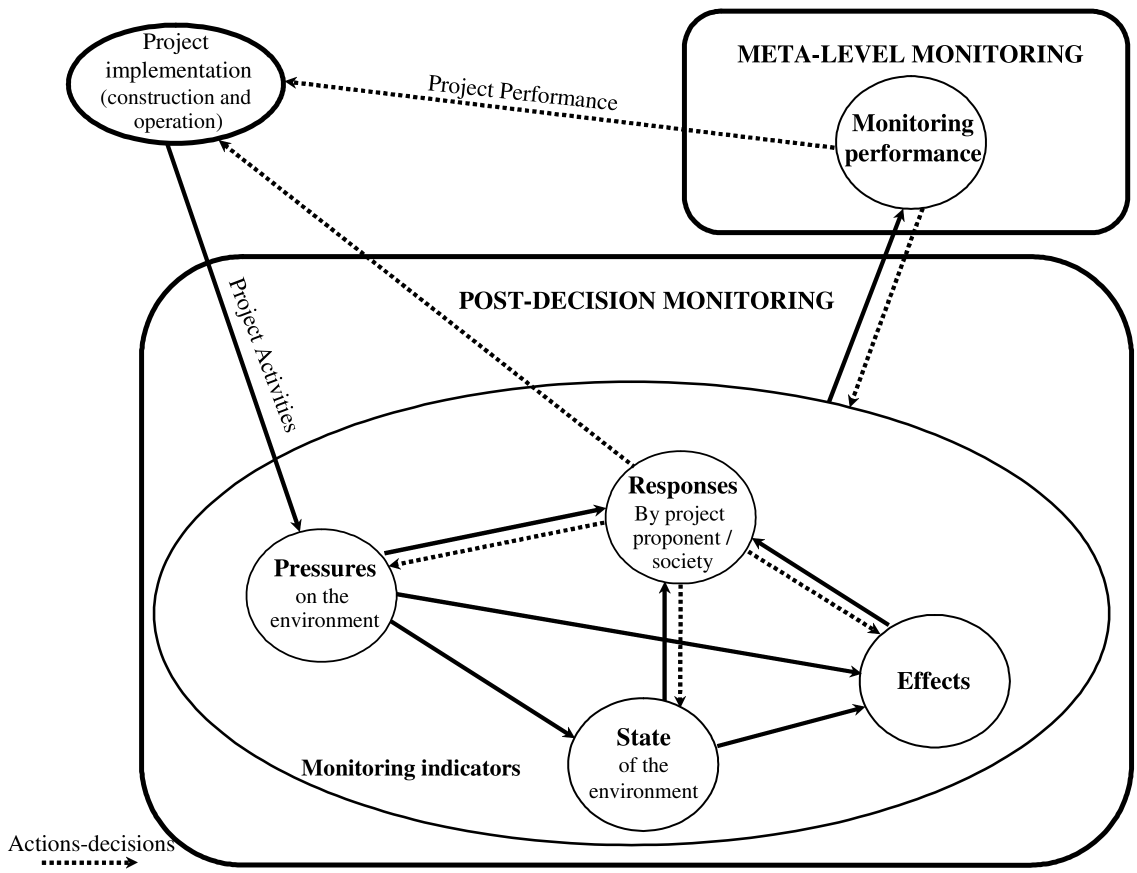

Figure I.2 – Environmental indicator framework to design and assess environmental post-decision monitoring programs – INDICAMP.

This framework was designed to cover the main stages of project implementation: (i) construction; (ii) operation; and (iii) decommissioning. Five fundamentals support monitoring indicator system development: (a) project type and dimension; (b) baseline environmental sensitivity; (c) major significant environmental impacts identified/predicted and related mitigation measures; (d) impacts which have poor accuracy or lack of basic data; (e) other environmental monitoring programs near the project area.

To relate the results from post-decision monitoring to the pre-decision monitoring a comparison is essential. The pre-decision monitoring could be ideally developed using the same *pressure, state, effects* and *response* categories, for a more efficient comparison, although the pressure indicators should consider the existing *pressures* without project.

Besides the main criteria presented above for monitoring indicator selection and development, various concepts, criteria and general guidelines must also be taken into account, namely those defined by Ott (1978), Barber (1994), UNEP/RIVM (1994), Ramos (1996), HMSO (1996) and Jackson *et al*. (2000). The implementation of INDICAMP therefore requires the definition of a set of indicators aimed at the different parts of the framework. Some of the most important criteria for indicator selection are:

- social and environmental relevance;
- ability to provide a representative picture of significant environmental impacts;
- simplicity, ease of interpretation and ability to show trends over time;
- responsiveness to change in the environment and related project actions;
- capacity to give early warning about irreversible trends;
- ability to be updated at regular intervals;
- present or future availability at a reasonable cost/benefit ratio;
- appropriateness of scales (temporal and spatial);
- acceptable levels of uncertainty;
- data collection methods comparable with other data sets;
- a good theoretical base in technical and scientific terms.
- existence of a target level or threshold against which to compare it so that users are able to assess the significance of the values associated with it;
- minimal environmental impact of the sampling process itself;

The development of environmental indicators is in most cases stimulated by information producers, with little involvement of information users. Therefore the adopted indicators should reflect the different perspectives of the EIA stakeholders. Morrison-Saunders *et al.* (2001) present and discuss the importance of stakeholders and their roles in the EIA follow-up and Noble (2000) emphasizes the importance of incorporating the public into all stages of the monitoring process.

In this framework, monitoring indicators can be aggregated into environmental indices, to reflect the composite monitoring results of each category of the framework. The aggregation functions (mathematical or heuristic) must be selected or developed for each particular case. Since there are many different functions with several advantages and disadvantages this step must be carried out with special caution to avoid significant losses of information and assure meaningful results.

To avoid a too complex and resource-demanding post-decision monitoring program, the INDICAMP indicators could be scored according to a qualitative expert knowledge assessment of their *relevancy* and *feasibility*. The *relevancy* classification covers: i) technical and scientific importance, ii) synthesis capability and iii) usefulness for communicating and reporting. The *feasibility* classification covers sensibility, robustness, cost and operability of the determination methods. In the first phase of the post-decision monitoring program only the indicators with the highest classification should be included. Each indicator is classified from 1 (lowest classification) to 3 (highest classification) and the more important indicators to use in INDICAMP should be the ones with a score of 6 (the sum of *relevancy* and *feasibility*). *Relevancy* should be the main criteria for indicators selection followed by the *feasibility* of the indicator determination method. The other scored indicators should be considered depending on a first results evaluation (Table I.2).

Overall indicators and their results should be reviewed periodically to identify opportunities to improve and achieve the monitoring objectives. Noble (2000) also stresses that an effective monitoring strategy must support the monitoring system designers in revising the monitoring design. One particular feature of this framework is the possibility of obtaining a significant part of the review information on the basis of the monitoring performance indicators. Some steps for the reviewing process can include a review of several points similar to those presented in ISO 14031 (ISO, 1999), namely: the appropriateness of the monitoring scope and objectives; the cost effectiveness and benefits achieved; progress towards meeting environmental criteria; the appropriateness of environmental criteria; the appropriateness of indicators; and data sources, data collection methods and data quality.

Table I.2 – Score of indicators according to their *relevancy* and *feasibility* (classified from 1 to 3).

Score	Relevancy	Feasibility
1st	3	3
2nd	3	2
3rd	3	1
4th	2	3
5th	2	2
6th	2	1
7th	1	3
8th	1	2
9th	1	1

I.4. COASTAL INFRASTRUCTURE AT THE SADO ESTUARY

Because mandatory post-decision monitoring is recent in Portuguese EIA regulations, few projects have developed and implemented monitoring programs. For this reason we choose to present a case study where the post-decision monitoring program was not implemented and where the indicators are selected and developed for the first time in this case study (see Table I.3). However this is a proposal to submit to local authorities as a decision-making support tool for project management in the estuary. Only the impacts on the aquatic system will be evaluated on this case study.

An EIS of the enlargement of a fishing harbor project was carried out in 1997. This harbor, with an area of 0.024 km^2, is located in the Sado estuary near the city of Setubal (Fig. I.3), and its enlargement was only concluded recently, in 2003. This enlargement aims at improving fishery conditions through the construction of an outside protection infrastructure and improvements in surrounding areas of the existing harbor.

Most of the estuary is classified as a nature reserve but also plays an important role in the local and national economy. The Setubal fishing harbor is located in the estuary's North Channel, under the direct influence of the Setubal urban area and upstream industries. Near the fishing harbor the Setubal urban sewage outfall is discharged and pleasure boat, fishing boat and ferryboat traffic is heavy. Near the project location, the Setubal and Sesimbra Harbours Administration has monitoring programs in the upper north and south channel prior to maintenance dredging works.

The Setubal fishing harbor enlargement will improve the uses of the aquatic system, in particular the fishery-related activities. Nevertheless, this project will have the typical significant negative impacts on the aquatic systems related with this type of infrastructure (see USEPA, 2001).

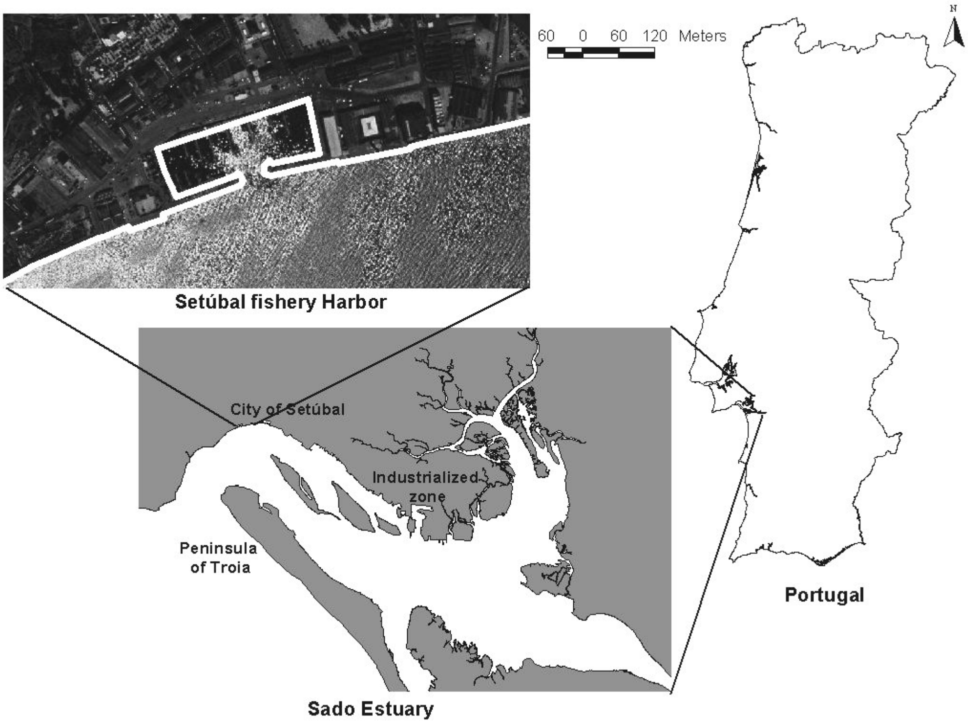

Figure I.3 – Setubal fishing harbor location in the Sado Estuary, Portugal (adapted from Caeiro *et al.*, 2003).

A set of indicators for each INDICAMP category was chosen to apply to the Setubal Fishing Harbor Enlargement Project. Some of these indicators were also chosen on the basis of USEPA (2001), EUROSTAT (1999) and ERM (1997) and of Portuguese and European environmental legislation.

Table I.3 lists the indicators chosen for five INDICAMP categories and attributes a score of 1 to 3 according to their *relevancy* and *feasibility*. In the first phase of the post-decision monitoring program only the indicators with a score of 6 will be included. The other indicators scored according to Table I.2 can be added to the monitoring program, depending on the first results campaign. During the monitoring reviews, adjustments should be made in order to respond to the results obtained. In this process the indicators not initially chosen, in accordance with the scoring previously established, should be taken into account. This ordering of indicator values makes this methodology less expensive and more effective.

Table I.3 – Indicators belonging to the INDICAMP categories and their score (from 1 to 3).

Indicators		**Relevancy**	**Feasibility**
Categories	**Units**		
Pressure			
Oil spill	kg/year	3	2
Fish discharge	tons live weight/year	3	3
Dredging operation	m^3/year	3	3
Dredge material disposal	m^3/year	3	3
Harbor pollution loads:			
- Discharges of domestic wastewater without suitable treatment	m^3 discharged/year	3	2
- Water runoff from harbor activities (boat operation, repair and maintenance, cleaning, fueling station, adjacent building areas, including parking) measured through modeling estimations	m^3/year	3	2
- Waste fish discharges	t/year	2	2
- Solid waste discharges	t/year	2	1
State			
Water quality:			
- pH		1	3
- Turbidity	m	3	3
- Dissolved oxygen	mg/l O_2	3	3
- Faecal contamination indicator	MPN/100 ml	3	3
- Nutrients (Nitrogen and phosphorus)	mg/l NH_4, N and PO_4	2	3
- Heavy metals: Zn, Cu, Cd, Pb, Ni, Cb and Cr	µg/l	3	3
- Polyaromatic hydrocarbons	µg/l	3	3
- Surfactants	mg/l	3	3
- Oils	mg/l	3	3
- Polychlorinated biphenyls	µg/l	3	3
- Organotin (TBT)	µg/l	2	3
- Debris and litter	nº/ m^2	3	3
Sediment quality			
- Faecal contamination indicator	MPN/100 mg	2	3
- Organic matter	%	3	3
- Redox potential	mV	3	3
- Heavy metals: Zn, Cu, Cd, Pb, Ni, Cb and Cr	µg/g	3	2
- Polyaromatic hydrocarbons	µg/g	3	2
- Polychlorinated biphenyls	µg/g	3	2
- TBT	µg/g	2	2
Macrozoobenthic community structure (assessed through species richness, abundance, biomass, species diversity, evenness, and *k*-dominance curves, among others)		3	1
Effects			
Sediment quality assessment (e.g. toxicity tests, macrozoobenthic communities disturbance assessment, Sediment Background Approach, Sediment Quality Triad Approach, Equilibrium Partitioning Approach)		3	2/1
Effects on the quality of organisms used in human diet:			
- presence of faecal contamination in bivalvia	MPN indicator of faecal contamination/g FW	3	3
- ictiofauna deformations	% deformations in vertebrae or ural plates	1	3
- molluscs/crustaceans, bioaccumulation of cont.	µg contaminant/g FW	3	2
- bivalvia, biotoxines accumulation	µg biotoxine /100 g FW	2	2
Organism mortality – fish	visual inspection of the number of deaths/species/year caused by project activities	3	3
Beach quality	number of beaches with bad quality water/year	2	2

Table I.3 – Indicators belonging to the INDICAMP categories and their score (from 1 to 3) (cont.).

Indicators: Categories	Indicators: Units	Relevancy	Feasibility
Responses			
Environmental law compliance	e.g. Nitrate, Water Framework and Sewage Sludge Directives (yes/no) or % regulatory requirements enforced	3	3
Dredging management program	e.g. m^3 of dredged material under management program	3	3
Waste management program	e.g. % of solid waste collected in appropriate containers	3	3
Waste water and water runoff management program	e.g. % of heavy metals removed by runoff control systems, like filtering practices	3	2
Boat washing and repair management program	e.g. % of boats washed without using toxic cleaners	3	3
Fueling station and petroleum control management program	e.g. oil spills near fueling station	3	3
Fish waste management control	e.g. % of fish reused as bait	3	2
Monitoring performance indicators			
Training personnel	no. persons allocated to the monitoring program submitted to environmental monitoring training courses	3	3
Monitoring investments and expenses	10^3 euros/Environmental Component of the Monitoring Program (ECMP)	3	3
Environmental monitoring activities	no. of sampling monitoring campaigns/ECMP	3	3
Institutional cooperation with other monitoring activities	no./ECMP	3	3
Harbor monitoring staff with environmental diary tasks	no. of persons/ECMP	3	3
Environmental education and awareness campaigns	no. of citizens/voluntary ECMP campaigns	3	3
Stakeholders' feedback to monitoring information	no. of messages received by mail/ECMP	3	2
Monitoring reporting and communication to stakeholders	reports; workshops; Internet; e-mail lists/ECMP	3	3
Average cost of monitoring indicator	euros/indicators used in ECMP	3	3
Chemical use in monitoring activities	e.g. loads of monitoring reagents reaching harbor waters/ECMP	3	2
Use of environmentally preferable products and equipment in monitoring activities	no. of environmentally preferable products /ECMP	3	2
Identification of unexpected environmental impacts under EIS	no./ECMP	3	2
Monitoring results used to validate impact prediction methods	no. of predictions methods validated/ECMP	3	2
Effectiveness of mitigation measures	no. of mitigation measures redesigned/ECMP	3	3
Implementation of environmental practices on the basis of monitoring results	no./ECMP	3	3
Analytical measurements and related detection levels	e.g. no. of indicator measurements under analytical detection level/ECMP	3	3

Some of the *pressure*, *state*, *effects* and *responses* indicators although with high relevancy classification have low feasibility classification due to high determination costs and/or difficult operability (e.g. macrozoobenthic community structure or sediment quality assessment). For that reason they should only be measured after first monitoring results evaluation. In the case of the monitoring performance indicators almost all of them have a maximum classification in terms of *relevancy* and *feasibility*. This does not mean that more effort is put into *monitoring performance* indicators, only that they are easier and less expensive to quantify.

The indicators belonging to the above categories could be produced by classification and aggregation of one or more indicators, by means of mathematical or heuristic algorithms. For example, the Pollution Load Index is calculated through the aggregation of contaminants like heavy metals or polyaromatic hydrocarbons. For a review of these and other indicators see for example Ramos (1996).

An in-depth analysis of the indicators listed above shows the difficulties that arise in the application of the INDICAMP framework to complex environmental problems, as with the case of marine resources. These difficulties may be due to several factors such as (Ramos, 1996; Antunes and Santos, 1999):

a. several causes contributing to a single effect;
b. multiple effects resulting from a single pressure;
c. interrelations among ecosystem components;
d. indirect, synergistic or cumulative effects;
e. identification of the mathematical equations that best represent parameter behavior.

One of the difficulties in accomplishing monitoring objectives is to assess whether the environmental changes observed are caused by that specific project or activity or whether other factors have intervened. The difficulties with causality can be problematic when, on the basis of the monitoring results, an authority decides that mitigation measures have to be taken. Besides, the environmental problems may not originate from a single activity but from the cumulative processes and synergetic effects of the combined polluting activities in an area. In that event, the mitigation measures implemented as part of the EIA follow-up of a single project can only be partial solutions to the environmental problems in an area that need concerted action. Nevertheless, an integrated area-oriented approach can help to identify the cumulative and synergetic character of environmental problems, since the total impact of the various activities in an area is monitored. That is why it is important to be aware of other monitoring programs in the study area. Furthermore, methodological problems of causality are less relevant to area-oriented monitoring because the state of the environment in a particular area and the environmental changes taking place there can usually be adequately assessed on and compared with, the prevailing environmental policy for that area (Arts *et al.,* 2000).

This post-monitoring approach attempts to measure project pressures (e.g. harbor pollution loads) and focuses on the timely prevention, restriction or remediation of environmental damage. This strategy identifies the pollution source instead of only evaluating the impact on the state of the environment and, thus, may avoid some serious problems relating to causality, as Arts *et al*., (2000) argue.

Like the PSR framework (OECD, 1993), INDICAMP tends to suggest linear relationships in project activities/environmental effects. This should not, however, obstruct the view of more complex relationships between project pressures and environmental-impact interactions. The INDICAMP framework does not attempt to make one-to-one linkages between specific *pressures*, environmental changes and *responses*. The *state* of the environment depends on the total *effects* of multiple *pressures*. As stressed by USEPA (1995), diagnosis of the causes of particular environmental or societal changes is usually difficult and multiple causation is the norm rather the exception. One way to deal with this complexity when designing monitoring programs is to avoid analyze unique linkages, and try to adopt an integrated approach, that relates different indicators as clusters with multiple aspects that interact with each other.

I.5. CONCLUSIONS

Post-decision monitoring is an essential step in the EIA process if the predicted impacts, the efficiency of mitigation measures and the shortcomings of prediction methods, measures and even regulations are to be verified and EIA practice improved. However, post-decision monitoring programs within EIA are fairly undeveloped compared to the pre-decision stages, as various problems arise at this stage, particularly related to financial and time constraints and proponent negligence.

Environmental indicators could contribute to designing and evaluating monitoring programs, thus improving establishment of the cause-effect relationship and the reporting and communication of environmental data, as the early-warning signals of a prevention strategy.

Based on the environmental indicator frameworks PSR/E, DPSIR and ISO 14031, a conceptual methodology to design and assess post-decision monitoring programs - INDICAMP – has been presented and discussed. This tool allows the incorporation of a systems analysis approach and the identification of the main cause-effect relationships between the different categories of monitoring indicators. A remaining issue of EIA follow-up is to assure the effectiveness of monitoring programs. To accomplish this a performance assessment tool such as the one included in the INDICAMP method appears to be useful. Moreover, the use of INDICAMP within EIA follow-up could contribute to increasing research activity in this domain. The case study showed examples of the indicators belonging to the different categories and also illustrated the benefits and drawbacks of the INDICAMP framework. Some difficulties arise in choosing the indicators for each category and in finding system interactions. Despite this, it seeks to represent an area-oriented approach, focus on prevention and find simple relationships in project activities/environmental effects. Multiple causalities have also to be analyzed to diagnose the causes of particular environmental or societal changes.

The baseline monitoring data and the preconditions to support the INDICAMP monitoring-indicators system are fundamental to assure that the Pressure, State, Effects and Responses categories assess project activities, and not other activities.

This framework could be adapted to other kinds of environmental monitoring programs, thus making the reporting of monitoring data easier for the general public.

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ANNEX II – INTEGRATION OF NUMERICAL MODELS IN GEOGRAPHIC DATABASES: THE CASE OF THE SADO ESTUARY MANAGEMENT

INTEGRATION OF NUMERICAL MODELS IN GEOGRAPHIC DATABASES: THE CASE OF THE SADO ESTUARY MANAGEMENT

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ABSTRACT

Geographic information systems (GIS) are now widely applied in coastal resource management. Their ability to organize and interface information from a large range of public and private data sources, and their ability to combine this information, using management criteria to develop a comprehensive picture of the system explains the success of GIS in this area. The use of numerical models as a tool to improve coastal management is also widespread. Less usual is a GIS-based management tool implementing a comprehensive management model and integrating a numerical modeling system into itself. In this paper such a methodology is proposed. A GIS-based management tool based on the DPSIR model is presented. An overview of the MOHID numerical modeling system is given and the method of integrating this model in the management tool is described. This system is applied to the Sado Estuary (Portugal). Some preliminary results of the integration are presented, demonstrating the capabilities of the management system.

KEYWORDS: numerical models, GIS, estuary management, DPSIR model.

II.1 INTRODUCTION

It is always a challenge to find the best methodology to manage complex and transition ecosystems like estuaries where the pressure of development is high.

The implementation of data management frameworks in coastal zones can be very useful in the start-up phase of management initiatives. The DPSIR methodology, developed by the European Environmental Agency, provides a framework for data synthesis and links environmental information using indicators. This model is being used with success in several programs (EEA, 1999a, EEA, 1999b), as well as other studies applied to oceans (Antunes and Santos, 1999), and coastal zones (*e.g.* Turner and Salomons, 1999, Turner, 2000).

GIS is being widely applied in coastal resource management. The need for some means of organizing and interfacing information from a large range of public and private data sources to develop a comprehensive picture of what is happening in the coastal zone has been recognized by resource managers (Ricketts, 1992).

The importance of hydrodynamic, transport and ecological models as decision-making tools has long been recognized. For an efficient management procedure it is essential to identify the current state of the system, to understand the basic mechanisms and interrelations between the different state variables, and to be able to predict the trends as a function of the management actions. A numerical modeling system can help to satisfy all these requirements. Data produced by the model must, however, be used within the framework of the management policy being implemented. This data must therefore be linked and crossed with data from a multitude of other sources. Data from a number of different sources is also needed to run the numerical model. This data is needed in the form of initial conditions, forcing functions, calibration and validation sets. External data, not relevant to the simulation itself, is also needed to understand the results and to interpret the processes. Traditionally these modeling systems run as independent units. The disadvantages of this approach are evident: the fluxes of information between the modeling system and the management tool are complex, due to their lack of compatibility. The need for special training in its interpretation will be a barrier to the information and lead to misjudgments. In this paper the 3D hydrodynamic and ecological modeling system MOHID is integrated into a management tool and applied to the Sado Estuary. The management tool is based on the DPSIR framework, implemented using a GIS. The modelling results will be integrated with the other data in the management tool, enabeling comparison and cross referencing of the whole data. A prototype of the integration of the transport model into the GIS management tool is demonstrated.

II.2 STUDY AREA

The Sado Estuary is the second largest estuary in Portugal with an area of approximately 24,000 hectares. It is located on the west coast of Portugal, 45 km south of Lisbon. Most of the estuary is classified as a nature reserve. Exception is made for the city of Setúbal, its port, and a considerable part of its surrounding area. The Sado Estuary basin is subject to intensive land-use practices and plays an important role in the local and national economy. Most of the activities in the estuary (e.g. industry, shipping, intensive farming, tourism and urban development) have negative effects on water, sediment and biotic communities (Caeiro *et al.*, 1999). The difficulties of the reserve authorities in managing urban growth are reflected in the higher urban growth rate inside the protected area boundary in comparison to its surroundings (Painho *et al.*, 1999). This is probably due to the fact that numerous official bodies are responsible for land-use planning in the reserve area, causing, at times, management deadlock.

II.3 DYNAMIC AND ECOLOGICAL MODEL

The Mohid modeling system is composed of a number of modules simulating hydrodynamic, sediment transport, water quality and ecological processes. The models are integrated using an object-oriented methodology (Miranda *et al.*, 2000).

The hydrodynamic model solves the three-dimensional incompressible primitive equations (Martins *et al.*, 1998, Martins *et al.*, 2001). Hydrostatic equilibrium is assumed as well as Boussinesq approximation. The specific mass is calculated as a function of temperature and salinity by a simplified equation of state. The model uses a finite volume approach. This method makes the solution independent of the mesh geometry, allowing the use of a generic vertical mesh. The horizontal mesh is the Arakawa-C staggered grid. The temporal discretization is carried out by means of a semi-implicit (ADI) algorithm with two time levels per iteration. The vertical eddy viscosity is calculated using the GOTM closures. The model also solves a transport equation for salinity and temperature in order to compute the specific mass. The Eulerian transport module used to transport these properties is based on the same finite volume method of the hydrodynamic model and is independent of the property transported. The same transport module is invoked in the sediment transport, water quality and ecological modules to transport different conservative and non-conservative properties. The sediment transport model simulates cohesive and non-cohesive sediments using an Eulerian approach. The falling velocity is computed by the Dyer (1986) formulation and the bottom exchanges are computed by different formulations (Partheniades, 1965, Odd and Cooper, 1989).

The ecological model uses a zero-dimension formulation that enables the use of the same model with both the Lagrangian and the Eulerian transport models. With this method the model equations are implemented in the form of sources and sinks in the transport models. Those terms are written in a generic form and can be applied both to Eulerian cells and to

Lagrangian particles. The ecological model simulates the nitrogen cycle, the dissolved oxygen concentration, the biochemical oxygen demand, and the zooplankton and phytoplankton concentrations (Pina, 2001). The nitrogen species include the three main inorganic forms: ammonia, nitrate and nitrite and also three organic fractions: the dissolved refractory fraction, dissolved non-refractory fraction and particulate fraction.

II.4 DYNAMIC, ENVIRONMENTAL MANAGEMENT OF THE SADO ESTUARY

II.4.1 Method description

The management methodology is based on the DPSIR model and is developed within the context of a GIS (Fig. II.1). This framework organizes information in five different categories, as follows. *Driving forces* are the underlying causes of environmental problems. They refer to the needs of individuals and institutions, which lead to activities that exert *pressures* on the environment. These pressures modify the *state* of the environment (*e.g.* change in water quality and fish populations) and, in turn, these modifications may have an *impact* on ecosystems and on human well-being. Undesirable impacts lead to a *response* from society that results in the formulation of an environmental policy. The policy responses lead to changes in the DPSIR chain. Depending on the results achieved, further responses are formulated (Antunes and Santos, 1999).

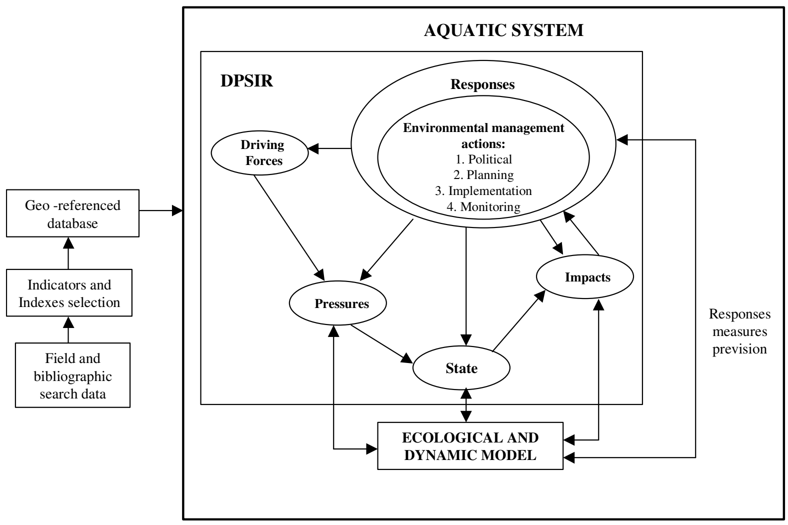

Figure II.1 - Sado Estuary management decision-making tool.

The identification and assessment of problems related to coastal zone environmental management therefore requires the definition of a set of indicators aimed at the different parts of the DPSIR framework. To permit its application to the Sado Estuary an appropriate set of indicators for each compartment were defined. This set was obtained by comparing optimal indicator selection, concepts and criteria against an extensive data search on the environmental characterization of the Sado Estuary (Caeiro *et al*., 1999).

In the proposed model, the state of the estuary is mostly evaluated through the sediment and benthos compartment. Sediment is a compartment where contaminants tend to accumulate first and suffer variations for short periods reflecting the average conditions of months. (*e.g* Wilson, 1988, Eliot and McManus, 1989, LUOMA, 1990). Also macrobenthic organisms are a primary means of assessing ecosystem response (Mucha and Costa, 1999). Studying the state of the estuary on the basis of the sediment and benthos compartment alone (not including the water compartment), also makes this methodology, easier to deal with, faster and more economical in terms of human and financial resources. These are essential factors in efficient environmental management.

This management tool is also based on identifying and characterizing a series of environmentally homogeneous sediment areas (management units). The boundary definition of each area was based on sediment general characterization parameters (fine fraction, redox potential and organic matter), strongly related to the composition and distribution of benthic organisms and contaminant mobility/accumulation. This data was collected in a campaign carried out from November 2000 to January 2001. 153 sites were sampled using a systematic unaligned sampling method (Webster, 1999) of a 500 x 750 m cell-size (Fig. II.2c) (Caeiro *et al.*, 2002). The boundaries of each homogeneous area were computed from data of the sediment parameters referred above and were defined through indicator kriging of cluster analysis based on the dissimilarity matrix function of geographical separation.

The environmental quality assessment of the estuary is performed by characterizing the indicators of the DPSIR categories in each management unit. The Sado Estuary environmental management area diagnosis is developed through different exploratory analyses, namely aggregation of indicators into different indices and statistical treatment. GIS will allow overlying the five different categories of the DPSIR model.

The integration of the ecological and dynamic model in the DPSIR framework allows useful outputs with this management tool. The sediment transport model calculates which estuary area will suffer an effect and resulting *impact* due to a certain *pressure* indicator.

Responses action forecast will also be possible using the ecological and dynamic model. These *Responses* measures will change the quantitative *pressure* indicator and resulting *state* and impact (Fig. II.1).

In summary, the dynamic modelling system will be introduced into this management tool in two ways: i) the management tool will be used as data input to the model and will be linked to one specific interface to run the model; ii) the model results will be integrated into the GIS database for analysis along with other information.

The integration between dynamic environmental and social economical data in the GIS allows the construction of a management support interface to end-users like the administration, the Nature Reserve, local authorities or private consultants. This management and planning tool is essential for the rehabilitation and recovery of the Sado Estuary zones already contaminated and for assuring the conservation and biodiversity of the protected areas.

II.4.2 Integration of the numeric model into the geographic database

The final objective of this work is to obtain a management tool able to drive the MOHID modelling system by itself. At that stage the management tool will be used to create the data needed by the modelling system and will be able to import the modelling results and merge them into its own structures for analysis. A step-by-step methodology is used to implement the integration. In the first step, reported in this paper, the model is driven outside the management tool. Only the model outputs are integrated.

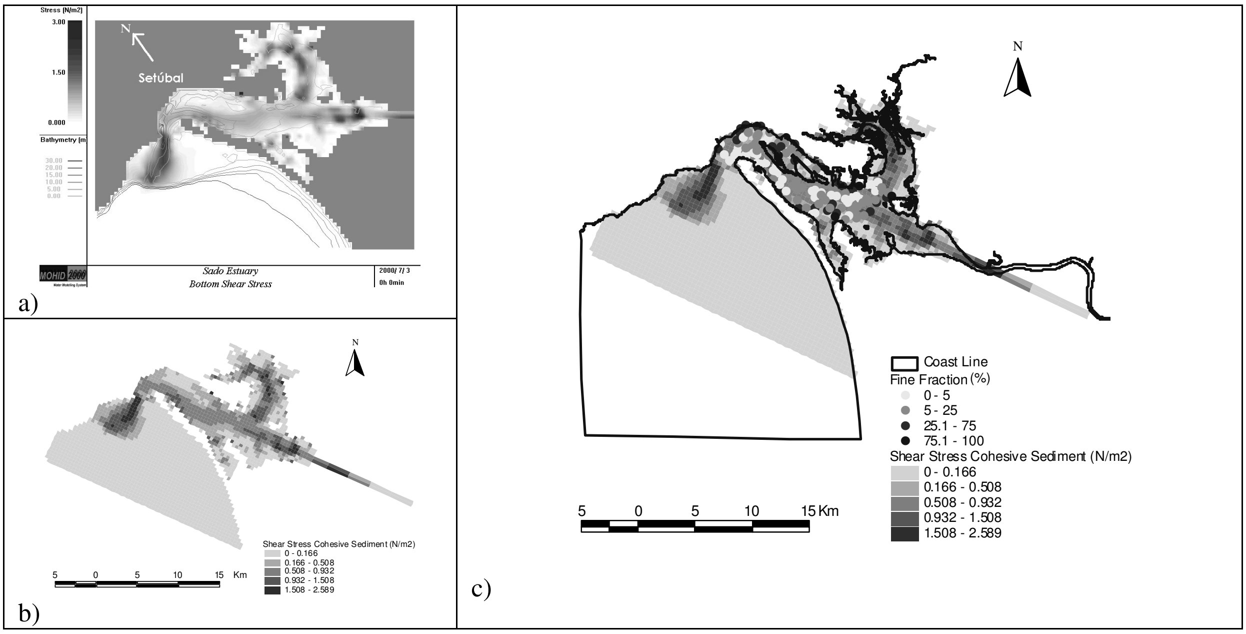

Figure II.2 - Bottom shear stress model results a) outside the GIS; b) inside the GIS; c) integrated with Sado estuary digitised boundaries and sediment fine fraction in 153 sampling sites.

The model results are produced in the *Hierarchical Data Format* (HDF) format. HDF was created at the National Center for Supercomputing Applications in the University of Illinois at Urban-Champaign, and is a multiobject file format for sharing scientific data in a distributed environment. HDF satisfies several requirements: support for types of data and metadata commonly used, efficient storage of and access to large data sets, platform independence and extensibility for future enhancements and compatibility with other standard formats.

At the first step of integration, several automatic procedures were developed to get information from the HDF files and produce files in a GIS format. The GIS file format adopted is the ESRI shapefile. These routines allow fast and easy integration of the files produced by the model in the management tool. The first routine extracts the matrix defined in the HDF file and creates a corresponding georeferenced layer. This process involves the shift of the original data to a new origin of coordinates and, after that, the rotation of the resulting layer. With these procedures a new georeferenced matrix is produced.

For each of the cells of the matrix we have a measure of a certain variable. The other routines get the variable values of the cells that are stored in the original HDF files and associating them to the corresponding cell in the georeferenced matrix.

An integration example of a transport model output into the GIS is shown in Fig. II.2. The integrated analysis of model results and field data in the GIS system is very powerful. In this example the correlation between higher shear stress areas and lower fine fraction sites are easily identified (Fig. II.2c).

The next step of the integration will allow the management tool direct access to the modeling system engine, eliminating the need for file format conversion and promoting full interaction between the modeling and management systems.

II.5 CONCLUSIONS

In this paper a method for integrating a 3D hydrodynamic and ecological model into a GIS estuary management tool was described. The prototype for the transport model integration into the GIS management tool shows how useful the interaction between this two systems is. This is specially true when combining model results with information from other different sources, which is essential for Sado Estuary management. Only first results were presented in this work. In the future the modelling system and the DPSIR management tool will be directly integrated into the GIS system.

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ANNEX III – SPATIAL SAMPLING DESIGN FOR MAPPING ESTUARINE MANAGEMENT AREAS: SUPPORT INFORMATION

SPATIAL SAMPLING DESIGN FOR MAPPING ESTUARINE MANAGEMENT AREAS: SUPPORT INFORMATION

Caeiro, S., Goovaerts, P., Painho, M., Costa, M. H. and Sousa, S. (2003)
Spatial sampling design for sediment quality assessment in estuaries. *Environmental Modelling and Software Journal* **18**(10) pp. 853 – 859.

III.1 EXPERIMENTAL SEMIVARIOGRAM ESTIMATION AND MODEL FITTING

From the sampled estuary area, only the sampling points with a smaller distance between them were used for semi-variograms computation (Fig. III.1). Big distances between sampling points could mask small-scale differences. According to Rodrigues and Quintino (1993) study, along the Sado estuary bay there are small areas of different granulometry, in particular in the North Channel, which should be taken into account in short-scale modelling. Therefore, for computation of the 120º direction semivariogram, 34 sampling points were used. In the 30º direction semivariogram, more sampling points were used (80) due to lack of lag pairs on that direction (See Table III.1). A lag distance equal to 0.25 km and angular tolerance equal to 30º was used for variography calculation. Less angular tolerance computed semivariograms with few lags and lag pairs and larger angular tolerance tended to underestimated anisotropy ratios. Less lag distance computed big differences between lags and longer lag distance computed bigger nugget effects. To better fit the semivariograms we eliminate the pairs of sites that were too distant from the slope of variance.

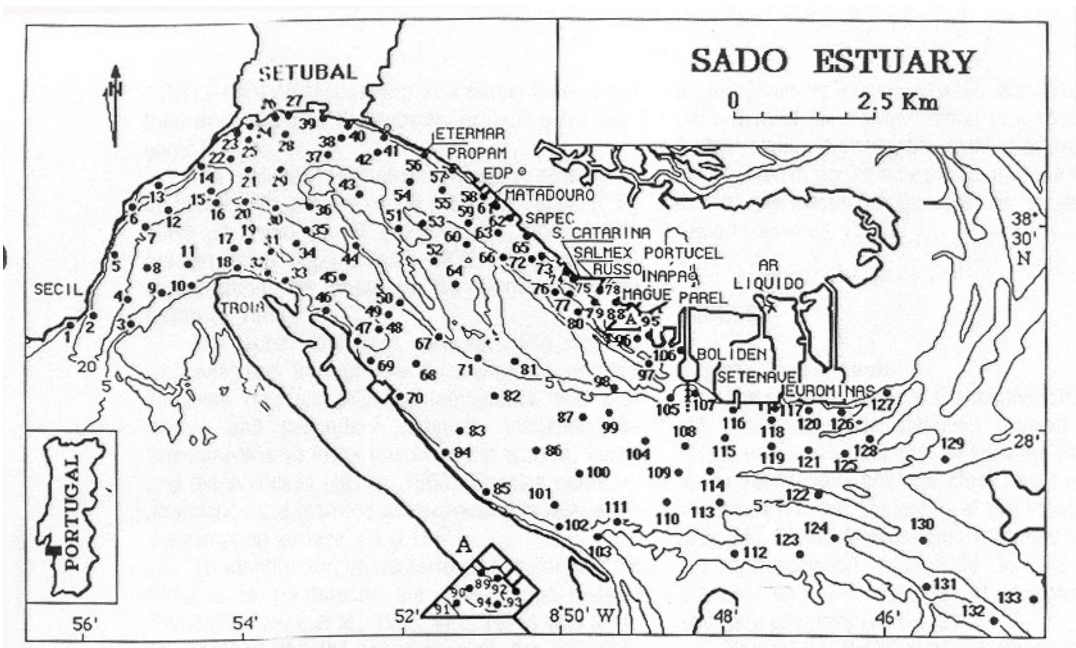

Figure III.1 – Sampling points from Rodrigues (1992) study.

Table III.1 –Sampling points and Fine Fraction (FF) values from Rodrigues (1992) study, used for grid unit length definition. Sampling points in bold used for 30º semivariogram computation and sampling points in italic used for 120º semivariogram computation.

Sampling points	FF (%)
1	**5,94**
2	**1,09**
3	**1,52**
4	**2,56**
5	**6,31**
6	**3,89**
7	**0,99**
8	**1,52**
9	**3,83**
10	**1,92**
11	**0,94**
12	**1,93**
13	**33,48**
14	**43,38**
15	**1,66**
16	**6,82**
17	**27,46**
18	**8,1**
19	**4,04**
20	**7,81**
21	**3,19**
22	**10**
23	**18,65**
24	**64,69**
25	**37,06**
26	**36,54**
27	**67,47**
28	**14,77**
29	**23,16**
30	**10,52**
31	**0,78**
32	**2,16**
33	**2,7**
34	**6,05**
35	**9,61**
36	**35,68**
37	**11,02**
38	**10,18**
39	**31,29**
40	**56,46**
41	**63,63**
42	**26,48**
43	**8,16**
44	**20,4**
45	**26,13**
46	**3,32**
47	**1,84**
48	**1,32**
49	**1,89**
50	**19,12**
51	**56,02**
52	**52,04**
53	**41,37**
54	***29,27***
55	***37,64***
56	***26,64***
57	***83,91***
58	***93,93***
59	***45,65***
60	***41,64***
61	***87,92***
62	***89,15***
63	***80,89***
64	**40,39**
65	***78,95***
66	***43,47***
67	**3,14**
68	**0,6**
69	**24,68**
70	**31,43**
71	**11,53**
72	***63,43***
73	***75,23***
74	***29,32***
75	***9,84***
76	***62,35***
77	***49,5***
78	***72,47***
79	***16,22***
80	***52,7***
81	6,29
82	35,78
83	7,56
84	12,42
85	37,33
86	12,91
87	28,92
88	*17,55*
91	*17,45*
92	*96,28*
95	*93,41*
96	*3,62*
97	*22,63*
98	13,67
99	7,57
100	28,72
101	30,4
102	93,75
103	22,33
104	2,77
105	19,92
106	*95,99*
107	*89,93*
108	6,83
109	27,72
110	26,28
111	27,54
112	22,23
113	29,09
114	22,6
115	1,7
116	*12*
117	*62,75*
118	*8,2*
119	1,59
120	*93,48*
121	13,12
122	32,9
123	2,41
124	26,22
125	*9,6*
126	*16,36*
127	1,93
128	7,86
129	24,01
130	47,07
131	5,38
132	48,07
133	84,02

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ANNEX IV – DELINEATION OF ESTUARINE MANAGEMENT AREAS USING MULTIVARIATE GEOSTATISTICS: SUPPORT INFORMATION

DELINEATION OF ESTUARINE MANAGEMENT AREAS USING MULTIVARIATE GEOSTATISTICS

– SUPPORT INFORMATION –

Caeiro, S., Goovaerts, P., Painho, M., Costa, M. H. *(2003)*

Environmental Science and Technology 37(18), 4052 – 4059.

Table IV.1 – Geographic coordinates Total Organic Matter (TOM), Fine Fraction (FF) and Redox Potential (E_h) and sampling date in the 153 Sampling points.

X (m)	Y (m)	Sampling station	Sampling number (cluster analysis)	% TOM	% FF	E_h (mV)	Sampling date
133199.7813	172748.8438	1	1	10.7	56.0	-391.0	31-10-2000
132801.7813	172432.0156	2	2	6.0	26.5	-298.3	31-10-2000
132385.6406	172048.8750	3	3	6.1	27.3	-330.0	31-10-2000
132016.5938	171730.1406	4	4	5.2	14.3	-189.1	18-01-2001
131529.6250	171565.7344	5	5	2.7	14.7	-196.2	31-10-2000
130980.1641	171065.6563	6	6	1.3	0.8	104.3	18-01-2001
130701.5391	170622.1094	7	7	7.1	63.8	69.3	18-01-2001
131308.6094	170200.1719	8	8	0.5	0.3	83.1	31-10-2000
131712.3438	169638.1250	9	9	0.7	0.5	92.6	31-10-2000
132196.3281	170124.4219	10	10	0.8	0.4	93.7	31-10-2000
132444.7500	170436.9844	11	11	0.7	0.4	108.5	31-10-2000
132494.2031	170785.9531	12	12	0.7	0.8	85.1	31-10-2000
132484.7188	171211.6406	13	13	2.2	13.6	-160.0	03-11-2000
132467.9844	171476.4688	14	14	5.7	33.8	-102.0	03-11-2000
132993.0156	171666.4375	15	15	1.0	3.9	-103.0	03-11-2000
133454.3125	172069.5625	16	16	2.3	8.9	-145.0	03-11-2000
134230.2969	172734.8125	17	17	6.9	39.4	-245.0	03-11-2000
134553.8125	172669.0625	18	18	9.0	44.7	-340.0	03-11-2000
134293.2344	172436.5781	19	19	6.9	34.9	-275.0	03-11-2000
134348.2813	172060.0625	20	20	4.9	17.6	-253.0	03-11-2000
134211.8750	171737.6406	21	21	2.9	12.5	-109.0	03-11-2000
134053.8906	171270.9844	22	22	3.5	15.7	-171.0	03-11-2000
133771.4375	170865.9063	23	23	1.3	6.1	-66.0	03-11-2000
133237.0781	170248.6563	24	24	0.7	0.5	137.0	03-11-2000
132665.9375	169937.0938	25	25	1.0	0.6	101.0	08-11-2000
132308.6250	169816.4375	26	26	0.6	0.4	104.0	08-11-2000
133145.7500	169933.0781	27	27	1.2	0.7	86.0	08-11-2000
133825.0938	170321.7031	28	28	0.6	0.6	98.0	08-11-2000
134263.5781	170597.5938	29	29	5.3	23.0	-109.0	08-11-2000
134411.9063	170951.6875	30	30	2.7	12.6	-172.0	08-11-2000
134938.8594	171381.8906	31	31	1.3	2.9	-137.0	08-11-2000
135261.2500	171703.2500	32	32	1.2	2.7	-160.0	08-11-2000
135294.1719	172174.7500	33	33	3.6	14.8	-239.0	08-11-2000
136769.8125	171648.4219	34	34	3.4	94.7	-324.0	08-11-2000
137539.0938	171111.3281	35	35	8.4	49.3	-299.0	10-11-2000
138036.6875	170404.4844	36	36	6.5	30.3	-202.0	10-11-2000
138859.3750	169806.1250	37	37	2.8	16.2	-166.0	10-11-2000
139677.7656	169372.6250	38	38	3.9	23.7	-223.0	10-11-2000
139937.4688	169094.9844	39	39	4.2	27.2	-192.0	10-11-2000
140298.7813	168805.5781	40	40	10.0	92.2	-294.0	10-11-2000
140827.8906	168177.8750	41	41	1.3	16.6	-86.0	10-11-2000
141534.3594	167529.0000	42	42	5.1	33.6	-251.0	10-11-2000
141827.2031	167386.2656	43	43	8.5	72.0	-149.0	15-10-2000
142746.2344	166955.7500	44	44	4.6	38.2	-164.2	17-01-2001
143052.7969	166500.4375	45	45	0.6	0.9	65.0	17-01-2001
144035.6875	166215.7188	46	46	2.1	10.2	-152.0	17-01-2001
144342.3906	165131.5938	47	47	3.9	28.6	-207.5	17-01-2001
143834.9531	164772.2188	52	48	1.2	6.3	-190.0	17-01-2001
143658.3906	165926.1563	53	49	2.0	10.8	-248.0	17-01-2001
142742.2813	165795.8594	54	50	1.2	6.6	-63.0	17-01-2001
142637.6250	166410.6563	55	51	0.5	1.4	-65.0	17-01-2001
142092.5156	166668.2344	56	52	0.9	7.0	-175.1	18-01-2001
141064.3438	167106.8281	57	53	2.5	11.1	74.0	10-11-2000
140456.5781	167531.4219	58	54	4.6	20.8	-399.0	10-11-2000
140365.8750	168037.3125	59	55	1.4	4.2	-145.0	10-11-2000
139830.7500	168448.2813	60	56	1.4	4.9	-224.0	10-11-2000
139535.7813	168872.2813	61	57	13.4	13.7	-164.0	10-11-2000
138733.5625	169511.0625	62	58	0.6	0.9	80.0	10-11-2000
137760.5938	170055.1250	63	59	2.4	12.4	-125.0	10-11-2000

Table IV.1 – Geographic coordinates Total Organic Matter (TOM), Fine Fraction (FF) and Redox Potential (E_h) and sampling date in the 153 Sampling points (cont.).

X (m)	Y (m)	Sampling station	Sampling number (cluster analysis)	% TOM	% FF	E_h (mV)	Sampling date
137302.8750	170660.0469	64	60	3.5	9.2	-166.0	10-11-2000
136735.5313	171173.5469	65	61	4.4	19.3	-175.0	08-11-2000
136300.0156	171620.8125	66	62	4.0	12.9	-210.0	08-11-2000
136122.5469	171242.7813	67	63	1.8	5.3	6.2	08-11-2000
136301.7031	170914.0000	68	64	5.6	29.1	-278.0	08-11-2000
136805.6094	170281.1250	69	65	3.9	14.8	-215.3	18-01-2001
137273.3438	169119.2031	70	66	2.1	10.5	-177.0	18-01-2001
139800.8594	167758.2188	72	67	4.3	22.4	-226.0	13-12-2000
141019.9219	166996.2031	73	68	3.3	12.1	-164.9	11-01-2001
142388.3125	166131.2500	74	69	0.9	0.7	50.5	18-01-2001
142095.0469	166222.2969	75	70	1.5	2.0	-168.2	18-01-2001
142289.5156	165946.9063	76	71	0.6	1.6	55.0	17-01-2001
142658.4219	165245.0938	77	72	2.5	18.4	-147.0	17-01-2001
143184.9531	165639.0000	78	73	3.7	22.3	9.8	17-01-2001
143101.4063	164529.6563	79	74	1.6	11.8	-170.0	17-01-2001
139655.6875	167413.3281	80	75	3.6	15.0	-126.0	13-12-2000
142434.3125	164839.7344	81	76	0.8	1.4	51.6	17-01-2001
141804.7188	165491.7813	82	77	2.5	12.0	-27.0	17-01-2001
140947.1094	165799.5625	83	78	3.8	26.8	-210.0	11-01-2001
141259.2969	166518.8906	84	79	0.9	1.6	62.4	11-01-2001
140823.4531	166596.2031	85	80	0.7	1.0	114.5	11-01-2001
139442.1406	167063.4531	86	81	1.4	5.0	-192.0	13-12-2000
137541.7656	168465.7813	87	82	1.3	1.2	28.0	18-01-2001
137613.3750	169645.4844	88	83	1.3	49.5	-213.9	18-01-2001
136091.9219	170136.8750	89	84	10.0	76.5	-242.1	18-01-2001
135900.3125	170532.2500	90	85	8.7	48.7	-225.0	08-11-2000
135578.9688	170901.1406	91	86	5.8	36.0	-230.0	08-11-2000
133148.5313	170795.2813	92	87	4.0	13.1	-223.4	16-11-2000
137394.6250	168442.7969	93	88	2.2	7.6	-40.0	13-12-2000
137902.0469	168231.7656	94	89	2.7	9.8	-65.0	13-12-2000
138887.4688	167761.3281	95	90	1.6	7.5	-126.0	13-12-2000
140000.8125	166886.8906	97	91	0.8	1.7	54.0	13-12-2000
140314.2969	166205.7031	98	92	2.7	13.3	-127.1	11-01-2001
140856.9063	165602.4688	99	93	4.4	38.9	-215.3	11-01-2001
141319.9375	165056.5781	100	94	5.6	32.9	-221.0	17-01-2001
142041.9063	164490.6563	101	95	1.1	6.4	-193.5	17-01-2001
141240.1719	164690.8594	102	96	9.1	81.4	-317.0	17-01-2001
140707.3438	165448.1563	103	97	3.6	20.6	-213.8	11-01-2001
139767.1719	165788.0156	104	98	3.3	15.7	-180.4	11-01-2001
139903.8438	166553.0625	105	99	4.2	11.4	-149.0	13-12-2000
139164.9063	166945.2813	106	100	0.9	2.9	47.0	13-12-2000
138214.9844	167328.1719	107	101	2.5	10.2	-270.0	13-12-2000
137726.9063	167775.7656	108	102	2.2	8.7	-60.0	13-12-2000
136935.1875	168276.1563	109	103	2.3	6.0	-145.0	13-12-2000
136242.3125	168938.4688	110	104	6.0	20.6	-60.0	13-12-2000
135948.3438	169088.6094	111	105	1.6	4.5	176.1	16-11-2000
135199.7344	169848.0156	112	106	0.7	0.4	104.6	16-11-2000
134437.6406	170547.8906	113	107	2.4	6.9	-134.2	16-11-2000
134219.6719	170214.7031	114	108	0.5	0.3	144.3	16-11-2000
134988.1406	169396.1719	115	109	1.0	1.5	12.0	16-11-2000
135673.9531	168793.0938	116	110	0.9	0.6	144.3	16-11-2000
136064.5781	168532.9063	117	111	1.1	1.3	45.0	13-12-2000
136489.4375	168001.8750	118	112	0.8	1.3	2.0	13-12-2000
137415.9219	167439.8125	119	113	2.6	8.2	-218.0	13-12-2000
137760.3125	167018.7344	120	114	2.0	8.4	-130.0	13-12-2000
138886.5313	166688.2188	121	115	4.4	13.6	-172.0	13-12-2000
139364.5000	166416.5313	122	116	1.5	4.6	46.0	13-12-2000
139419.7813	165446.3438	123	117	6.0	38.3	-162.4	11-01-2001
138984.3750	165205.7031	124	118	6.0	47.3	-204.4	11-01-2001
137901.2969	165502.4063	125	119	8.4	62.6	-302.3	17-11-2000
136936.5938	166231.5625	126	120	2.8	12.8	-323.7	17-11-2000
136281.9375	166962.1563	127	121	7.6	38.3	-201.0	17-11-2000
136079.7188	167145.0313	128	122	3.4	29.5	-220.2	17-11-2000
135864.0156	167461.4063	129	123	5.0	12.6	-175.1	17-11-2000
135620.4219	167910.9844	130	124	3.0	11.7	-184.0	17-11-2000
135109.8906	170425.9531	131	125	2.6	13.8	-243.9	16-11-2000
134217.6406	169430.4063	132	126	0.8	0.6	115.0	18-01-2001
134232.3594	169450.6250	133	117	0.9	2.8	54.7	16-11-2000
136184.5313	167523.6406	134	128	1.1	3.4	-163.1	17-11-2000
136747.6563	166995.3125	135	129	1.3	4.0	-194.4	17-11-2000
137864.1094	166150.2031	136	130	2.9	9.7	-158.2	17-11-2000

Table IV.1 – Geographic coordinates Total Organic Matter (TOM), Fine Fraction (FF) and Redox Potential (E_h) and sampling date in the 153 Sampling points (cont.).

X (m)	Y (m)	Sampling station	Sampling number (cluster analysis)	% TOM	% FF	E_h (mV)	Sampling date
138595.2188	165495.3750	137	131	4.4	13.6	-124.8	17-11-2000
139357.2344	165058.4688	138	132	0.8	0.8	100.0	17-11-2000
142782.5000	167336.6250	139	133	10.8	87.1	-256.8	15-10-2000
143397.6719	166301.9219	140	134	0.8	2.4	128.6	15-10-2000
144309.5469	166060.5156	141	135	3.8	10.7	-222.6	15-10-2000
144958.6250	165884.0938	142	136	4.3	29.3	25.2	15-10-2000
144751.2344	166181.1094	147	137	2.0	6.6	-103.2	15-10-2000
144796.9063	166915.5313	148	138	0.8	1.0	50.1	15-10-2000
144063.4063	167481.2969	149	139	1.3	2.5	39.9	15-10-2000
143365.7500	167345.6094	150	140	11.1	96.1	-268.7	15-10-2000
144510.0156	167493.0156	151	141	1.7	3.2	44.7	15-10-2000
145462.6719	166838.9844	152	142	5.0	22.7	-138.8	15-10-2000
145813.1563	166392.3750	153	143	5.4	26.2	-210.3	15-10-2000
145068.6875	167720.3906	154	144	0.7	2.1	44.4	15-10-2000
145367.0781	167331.7188	155	145	2.2	8.0	-149.0	15-10-2000
145870.0000	166847.2344	156	146	3.8	19.7	-94.3	15-10-2000
146293.9688	166507.7188	157	147	9.6	90.5	-198.6	15-10-2000
134580.1094	169297.8594	1110	148	1.0	1.9	164.1	16-11-2000
135522.9688	169906.3906	1111	149	3.2	14.5	-213.1	18-01-2001
135281.6094	170084.0781	1120	150	3.5	9.2	-230.2	16-11-2000
140527.0781	165264.4219	1230	151	5.6	34.1	-212.0	11-01-2001
139192.9375	164889.4844	1240	152	1.0	3.8	-9.0	17-11-2000
142964.3438	164900.3125	800	153	2.2	6.5	-101.4	17-01-2001

Table IV.2 – Squared Mahalanobis distance between clusters of method 1.

	Cluster 1	Cluster 2	Cluster 3	Cluster 4
Cluster 1	0	8.22	30.41	93.58
Cluster 2	8.22	0	7.48	46.79
Cluster 3	30.41	7.48	0	21.14
Cluster 4	93.58	46.79	21.14	0

Table IV.3 – Indicator semivariogram models for each cluster, see Eq. 4.1 for symbol significance.

			1st structure			2nd structure		
Property	c_o	Model	c	a_{max}	a_{min}	c	a_{max}	a_{min}
Cluster 1	0.002	Spherical	0.073	854	769	0.038	3721	3721
Cluster 2	0.117	Spherical	0.123	671	201	-	-	-
Cluster 3	0.068	Spherical	0.130	1098	1043	-	-	-
Cluster 4	0.092	Spherical	0.07	1520	1034	0.04	2135	1772

Table IV.4 – Semivariogram models for the three environmental attributes.

			1st structure			2nd structure		
Property	c_o	Model	c	a_{max}	a_{min}	c	a_{max}	a_{min}
Organic matter	0.2	Spherical	0.41	1304	1304	0.12	4035	2946
Fine fraction	0.32	Spherical	1.33	1400	1078	0.37	5490	1647
Redox potencial	4370	Spherical	13870	2266	2266	1900	1586	1396

Table IV.5 – Squared Mahalanobis distance between groups of method 2.

	Cluster 1	Cluster 2	Cluster 3	Cluster 4
Cluster 1	0	7.09	29.72	97.25
Cluster 2	7.09	0	7.97	53.56
Cluster 3	29.72	7.97	0	20.91
Cluster 4	97.25	53.56	20.91	0

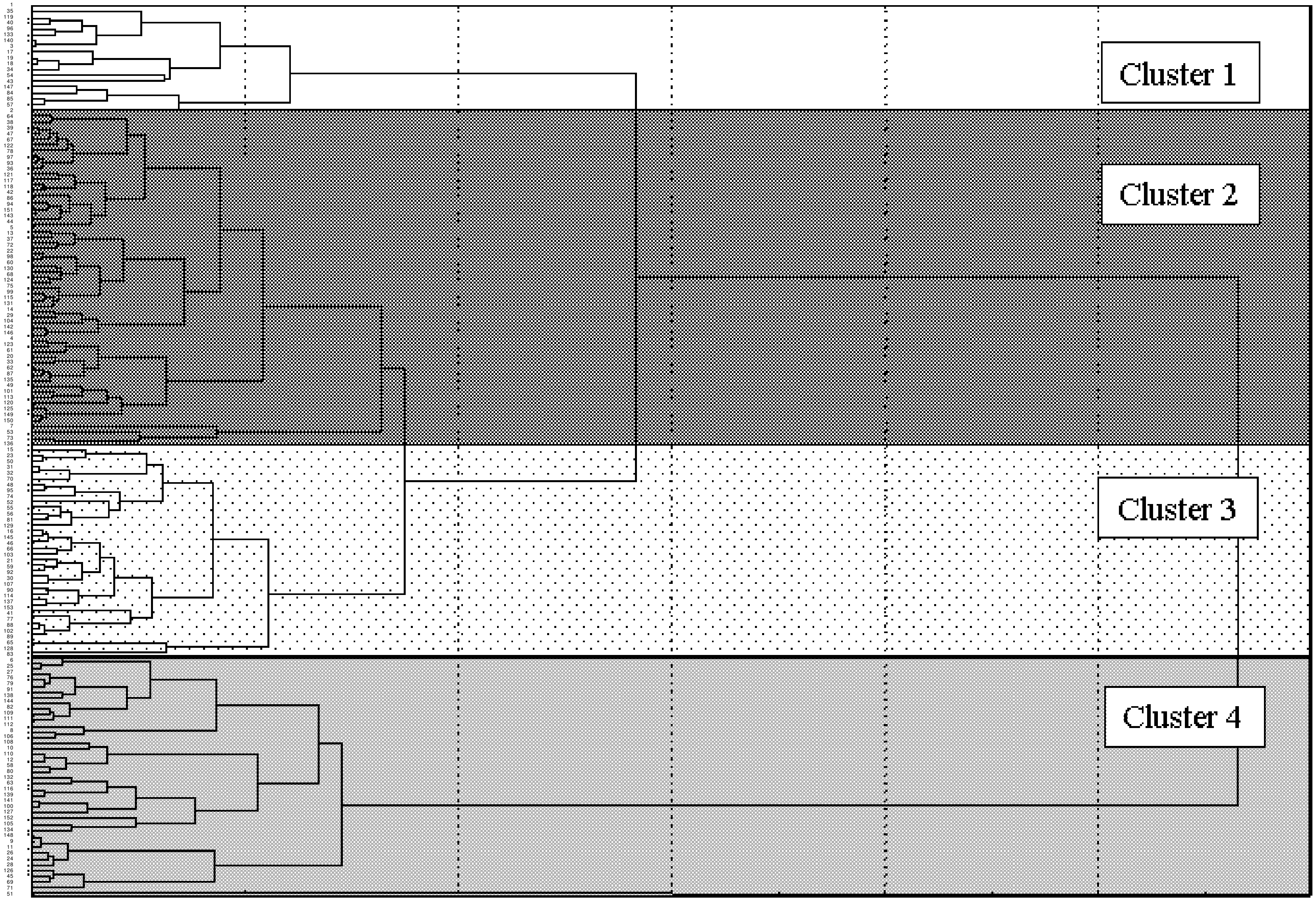


Figure IV.1 – Hierarchical classification (Euclidian distances with complete linkage rule) of dissimilarity matrix d_{ij}^{*} and 4 clusters yielded (method 1).

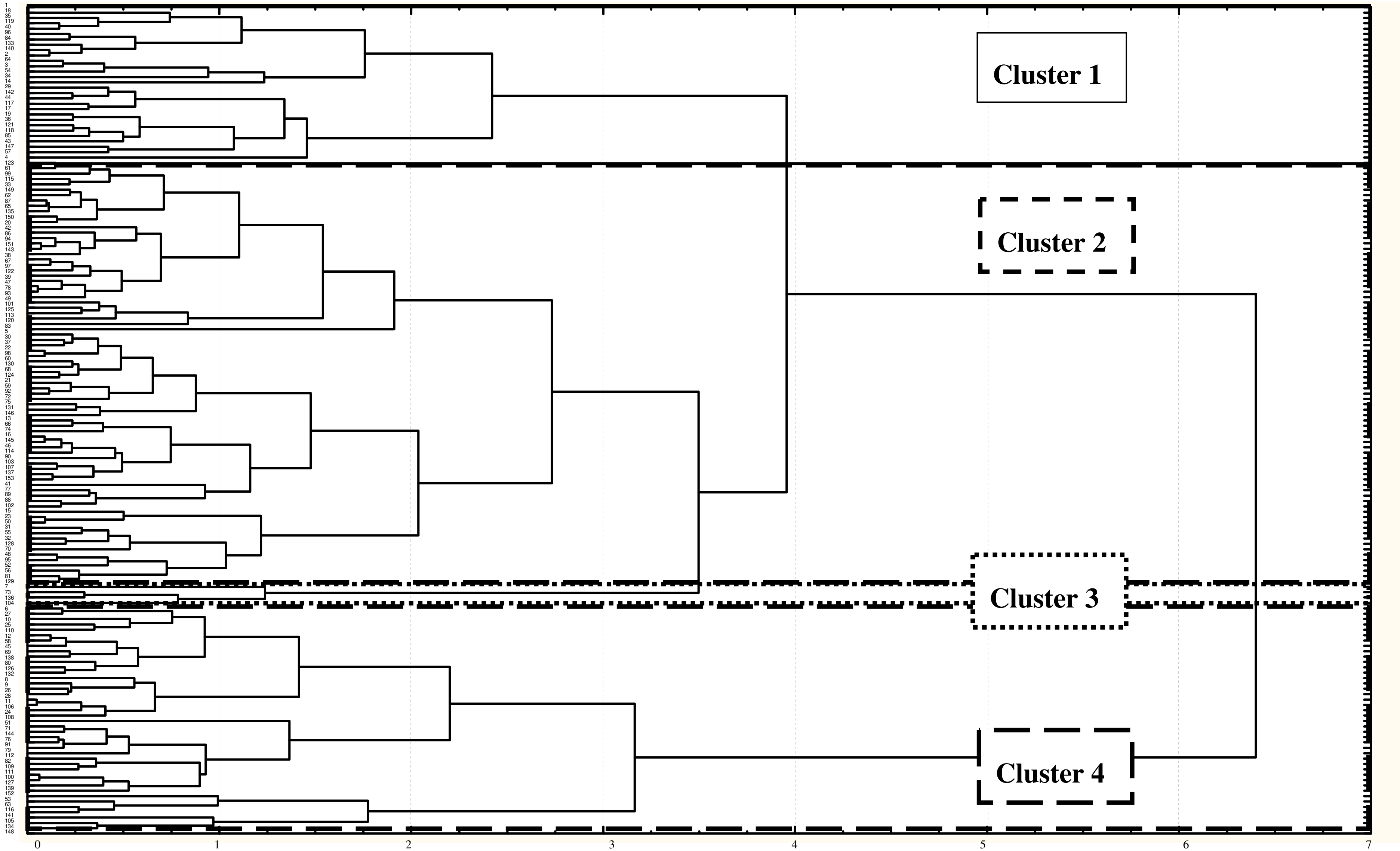


Figure IV.2 – Hierarchical classification (Euclidian distances with complete linkage rule) of d_{ij} and 4 clusters yielded (method 1.1).

GOOVAERTS AND WEBSTER (1994) PROCEDURE

To investigate the impact of accounting for geographical distances into the computation of the dissimilarity matrix, the methodology described in Goovaerts and Webster (1994) was used. A clustering tree based on the 3 attributes measured at the 153 sampling points was created with (spatially weighted classification – Fig. IV.1) and without (unweighted classification – Fig. IV.2) taking into account the spatial distance between sampling sites, i.e. with and without any modification of the dissimilarity matrix (d_{ij}). In both cases, the indicator semivariograms for each cluster were computed and combined according to equation IV.1, see Fig. IV.3. Each graph can be interpreted as the estimated probability that two observations, a distance *h* apart, belong to different clusters. The smaller the value of *p(h),* the better the spatial contiguity. For the first class of distance this probability is smaller for the classification that weights dissimilarity between observations according to their separation distance in the geographical space (d_{ij}^*).

$$p(h) = \sum_{l=1}^{L} \gamma(h; s_l) \qquad \text{(eq. IV.1)}$$

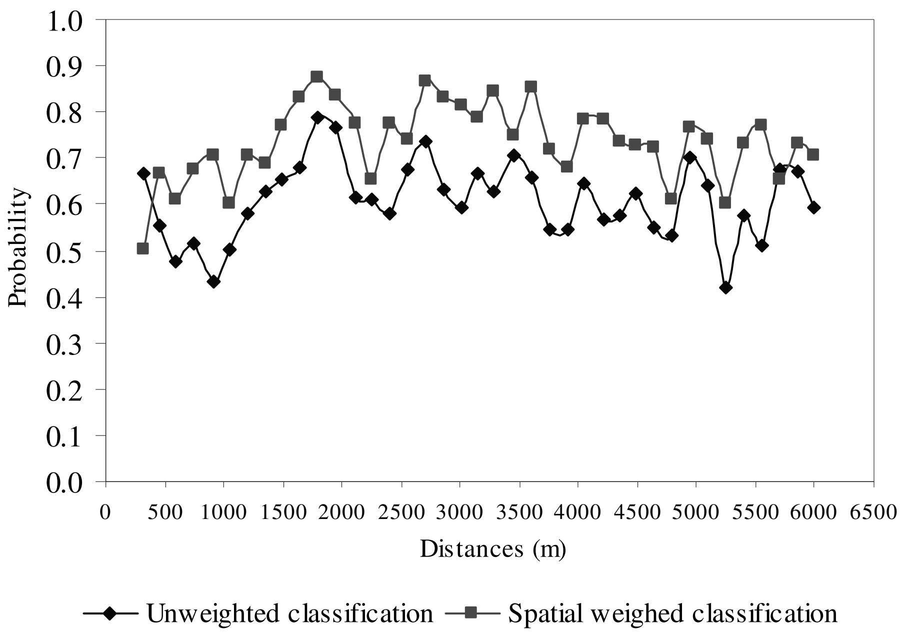


Figure IV.3 – Estimated probability that two sites belong to different clusters created using spatially weighted and unweighted classifications, against the distance *h*.

CROSS VALIDATION OF SEMIVARIOGRAMS MODELS USED IN METHOD 2

When adjusting the semivariogram model, Variowin software indicates the goodness of the fit by a weighted standardized measure, standardized by the variance of the data and weighted by the number of pairs in each lag and the inverse of the mean distance of the lag (Pannatier, 1996). However this automatic fit rarely provides definitive results, although is a first step of a manual fit (Chilès and Delfiner, 1999). Also, the objective of model adjustment is to capture the major spatial features of the attribute, not to build a semivariogram model that is the closest possible to experimental values (Goovaerts, 1997). It is then necessary to use validate measures in order to validate the consistency of the data with the assumed model. Cross validation techniques were then used to evaluate the impact of the semivariogram model on interpolation results (Goovaerts, 1997) (Table IV.6).

The models were the best fitted for FF, TOM and Eh attributes (Fig 4.6), compared to other model adjustments without outlier values or different fitted models. This choice was based on cross-validation techniques comparison and manual models adjustments, like minimum nugget effect/sill ratio and longest range. Also, the decision on the model was conducted according to our experience, information available and the objective of the study (Goovaerts, 1997).

The following cross-validation statistics were used in the models fitted (Amstrong, 1998):

i) Symmetry of errors distribution: average of the estimation errors should be near zero:

$E\left(Z_{\alpha}^{*} - Z_{\alpha}\right) = 0$, where Z_{α}^{*} is the estimate value and Z_{α} the true value (eq. IV.2)

ii) Mean of the standardized estimation errors: the average of the errors divided by estimation standard deviation should be zero:

$$E\left(\frac{Z_{\alpha}^{*} - Z_{\alpha}}{\sigma_{\alpha}}\right) = 0 \qquad \text{(eq. IV.3)}$$

iii) Variance of the standardized estimation errors: variance of the quotient between estimation errors and the standard deviation should be one:

$$Var\left(\frac{Z_{\alpha}^{*}-Z\alpha}{\sigma_{\alpha}}\right)=1 \qquad \text{(eq. IV.4)}$$

Also the selected models behavior were inspected by the analysis of the following plots:

iv) Scatergram of true values versus the estimated values (Deutsch and Journel, 1998): trend line should have 45º slope.

v) Scatergram of the errors $\left(Z_{\alpha}^{*}-Z_{\alpha}\right)$ versus the estimates value Z_{α}: the errors should be centered on zero error line (conditional unbiasedness) (Deutsch and Journel, 1998).

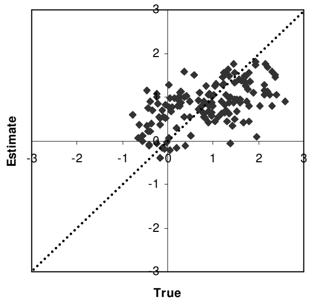
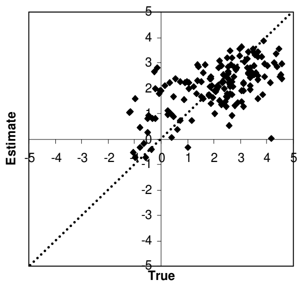
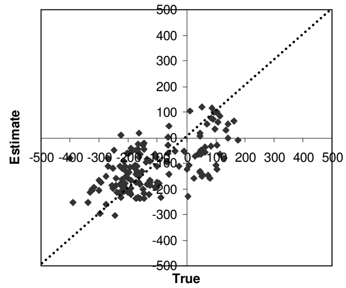
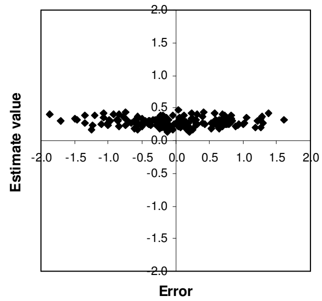
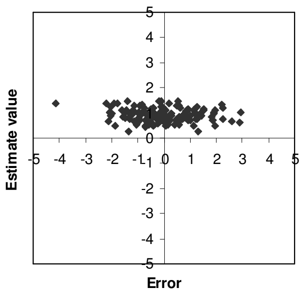
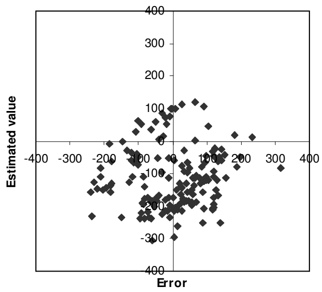
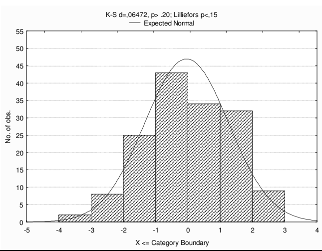
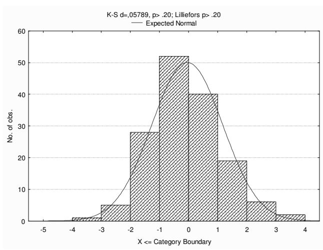
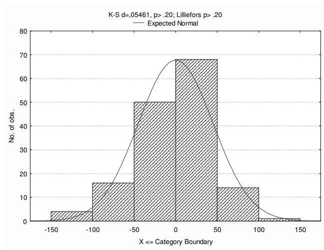
vi) Histogram of standardized errors: the errors should be considered Gaussian (Chilès and Delfiner, 1999).

These plots are meant to detect the presence of residual structure not accounted for the selected model and should be used qualitatively (Chilès and Delfiner, 1999).

The cross validation statistics (Table IV.6) showed that the 3 final models were acceptable at least for one of the statistics. No matter whether robust or ordinary statistics are used, is not common for all three statistics to show the same model as being "the best" (Amstrong, 1998). The plot of the true versus the estimated values exhibit the typical spatial smoothing of kriging (conditional bias), i.e. overestimation of low values and underestimation of high values (Isaaks and Srivastava, 1989 and Deutsch and Journel, 1998). The scatterplot of $\left(Z_{\alpha}^{*}-Z_{\alpha}\right), Z_{\alpha}^{*}$ indicates in general no major dependency of the error on the Z_{α}^{*} value (except for Eh attribute, in negative values). The histograms of standardized errors is symmetric around zero and Gaussian like.

Nevertheless special care must be taken when interpreting the cross-validation statistics and plots. This validation technique only tests the goodness of fit of the vertical component of the variogram and not the rest of the model (Amstrong, 1998). The best cross-validated results may not yield the best predictions at unsampled locations Also, cross-validation remove and re-estimates and the resulting kriged estimate depends mainly on the nearest samples (Isaaks and Srivastava, 1989, Goovaerts, 1997 and Chilès and Delfiner, 1999).

Table IV.6 – Cross validation results for the 3 attributes block kriging models.

Validation	TOM	FF	Eh
$E\left(Z_\alpha^* - Z_\alpha\right)$	-0.025	-0.058	2.2
$E\left(\frac{Z_\alpha^* - Z_\alpha}{\sigma_\alpha}\right)$	-0.04	-0.046	0.196
$Var\left(\frac{Z_\alpha^* - Z_\alpha}{\sigma_\alpha}\right)$	1.68	1.48	2034
Z_α^*, Z_α scatterplot			
$\left(Z_\alpha^* - Z_\alpha\right),\ Z_\alpha^*$ scatterplot			
$\frac{Z_\alpha^* - Z_\alpha}{\sigma_\alpha}$ histogram			

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ANNEX V – MAP SIMILARITY MEASUREMENT AND IT'S APPLICATION TO THE SADO ESTUARY: SUPPORT INFORMATION

ASSESSMENT OF MAP SIMILARITY OF CATEGORICAL MAPS USING KAPPA STATISTICS: THE CASE OF SADO ESTUARY

Sousa, S., Caeiro, S. and Painho, M. (2002)

Sousa, A. *et al.,* (Ed.). *Proceedings of ESIG 2002. VII Encontro de Utilizadores de Informação.* 13 – 15 Novembro, USIG, Oeiras, pp. 1- 6

ABSTRACT

In the past thirty years GIS technology has progressed from computer mapping to spatial database management, and more recently, to quantitative map analysis and modeling. However, most applications still rely on visual analysis for determining similarity within and among maps. The aim of this study is to compare management areas of Sado estuary (categorical maps) computed from three different interpolation methods. Different kappa statistics and visual map overlays were used for map comparison. The confusion matrix was used to calculate the Kappa coefficients, to assess agreement between the three interpolation methods. These map comparison techniques help to confirm the no gain of precision of one the methods for homogenous areas delineation and help to find the main sources of difference between the maps.

KEYWORDS: Comparison methods, assessment of map similarity, Kappa statistics

V.1.1 INTRODUCTION

In the different GIS applications, environmental in particular, compare or detect different categorical maps is an essential issue. The accuracy of a comparison procedure based on a more reliable and robust approach could have a marked improvement in the ability to detect a map change.

Map comparison procedures can express the similarity between two maps by looking at simple proportions of areas or by measuring it numerically. This numerical similarity could be assessed by categorical representation of overlay results as a contingency table, and statistical analysis of the latter with various integral measures of association, log-linear models, among others (Zaslavsky, 1995). The result of a map comparison can be an overall value for similarity (e.g a value between 0 and 1) or a map in it's own, which means that the result of a comparison of two maps is a third map which indicates per location how strong the similarity is (Hagen, 2002b).

In many situations, it is preferential to express the level of agreement in a single number. When the comparison consists of a number of pairwise comparisons, the kappa statistic can be a suitable approach (Carletta, 1996). The Kappa index of agreement for categorical data was developed by Cohen (1960) and was first used in the context of psychology and psychiatric diagnosis and was subsequently adopted by the remote sensing community as a useful measure of classification accuracy.

The aim of this study is to present some new variants of Kappa statistic introduced by Pontius (2000) and Hagen (2002b) and use them to compare three maps. These maps represent different methods of delineating environmental management areas of the Sado Estuary.

V.1.2 METHODS

In order to divide the Sado Estuary in homogenous areas for future environmental management of this ecosystem, geostatistical multivariate techniques were used. Three maps of final management units were computed from three sediment characterization indicators, using: 1) cluster analysis of dissimilarity matrix function of geographical separation followed by indicator kriging of the cluster data, 2) discriminant analysis of kriged values of the three sediment attributes, 3) combination of methods 1 and 2 (fig. V.1.1) (Caeiro *et al.,* 2003).

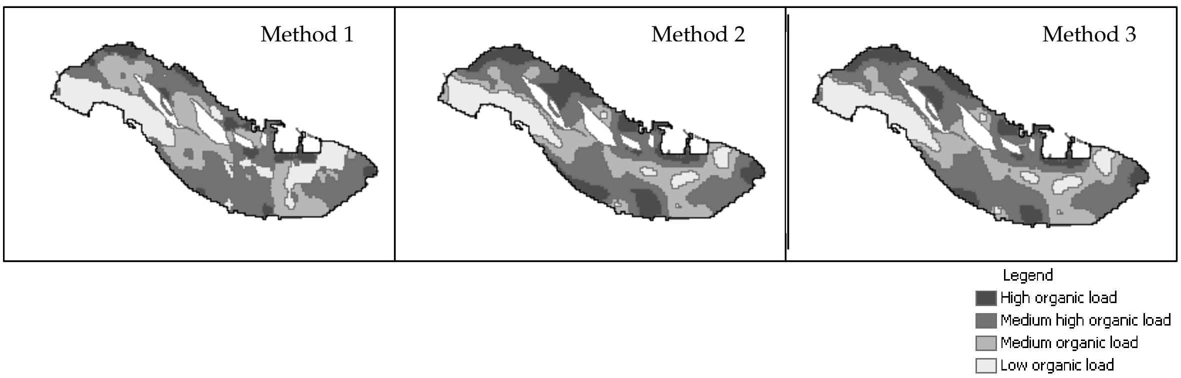

Figure V.1.1 – Maps representing the 3 methodologies for Sado estuary management areas delineation.

The aim of a pair wise post classification comparison is to identify areas of categorical disagreement between two maps by determining the pixels with a difference in theme. For that purpose maps were overlaid on a pixel-by-pixel basis to produce a map and attribute table of site specific differences using simple operations of map algebra in the "map calculator" and reclassify within Arc View®.

To express the level of agreement of the 3 maps in a single number Kappa statistics were used, based upon the so called contingency table (or confusion matrix) - Table V.1.1. This table details how the distribution of categories in map A differs from map B. p_{iT} is the proportion of cells of category i in map A, p_{Ti} is the proportion of cells of category *i* in map B and p_{ij} is the proportion of cells of category *i* of map A in category *j* of map B (Hagen, 2002b).

Table V.1.1 – The contingency table (Adapted from Monserud and Leemans, 1992).

Map A categories	**Map B categories**						**Total**
	1	2	*i*	*j*	.	c	
1	$\boldsymbol{p_{11}}$	p_{12}	p_{1i}	p_{1j}	.	p_{1c}	p_{1T}
2	p_{21}	$\boldsymbol{p_{22}}$	p_{2i}	p_{2j}	.	p_{2c}	p_{2T}
i	p_{i1}	p_{i2}	$\boldsymbol{p_{ii}}$	p_{ij}	.	p_{ic}	p_{iT}
j	p_{j1}	p_{j2}	p_{ji}	$\boldsymbol{p_{jj}}$	.	p_{jc}	p_{jT}
.	.	.	.	.	.	.	.
c	p_{c1}	p_{c2}	p_{ci}	p_{cj}	.	$\boldsymbol{p_{cc}}$	p_{cT}
Total	p_{T1}	p_{T2}	p_{Ti}	P_{Tj}		p_{Tc}	**1**

Three statistics derived from the contingency table were used (Hagen, 2002a):

"*P(A)* stands for Fraction of Agreement and is calculated according to equation (eq. V.1.1):

$$P(A) = \sum_{i=1}^{c} p_{ii} \qquad \text{(eq. V.1.1)}$$

P(E) stands for Expected Fraction of Agreement subject to the observed distribution, and is calculated according to equation (eq. V.1.2):

$$P(E) = \sum_{i=1}^{c} p_{iT} * p_{Ti} \qquad \text{(eq. V.1.2)}$$

P(max) stands for Maximum Fraction of Agreement subject to the observed distribution, that mean the maximum agreement that could be attained if the location of the cells in one of the maps was to be rearranged and is calculated according to equation (eq. V.1.3):

$$P(max)=\sum_{i=1}^{c} min(\, p_{iT}\,, p_{Ti}\,) \qquad \text{(eq. V.1.3)"}$$

These statistics were then used for Kappa calculation defined according to the following equation (eq. V.1.4) (Cohen, 1960):

$$K=\frac{P(A)-P(E)}{1-P(E)} \qquad \text{(eq. V.1.4)}$$

Kappa is the proportion of agreement *P(A)* after chance agreement *P(E)* has been removed. If kappa=1, there is perfect agreement. If kappa=0, the agreement is the same as would be expected by randomly arranging cells. The stronger the agreement is, the higher is the value of kappa. Negative values occur when agreement is weaker than expected by chance, but this rarely happens (Table V.1.2).

TableV.1.2 – Strength of agreement of maps comparison according to *Kappa* values (Landis, 1977).

***KAPPA* VALUES**	**Strength of Agreement**
< 0.00	poor
0.00 – 0.20	slight
0.21 – 0.40	fair
0.41 – 0.60	moderate
0.61 – 0.80	substantial
0.81 – 1.00	almost perfect

The reason to apply Kappa is that the total number of cells taken in by the individual categories can explain part of the cell-by-cell agreement between two maps. Nevertheless Pontius (2000), clarifies that Kappa statistic confounds quantification error with location error and introduces two statistics to separately consider similarity of location and similarity of quantity.

Klocation compares the actual success rate to the expected success rate relative to the maximum success rate given that the total number of cells of each category does not change.

The maximum success rate is calculated according to equation (eq. V.1.3) and Klocation according to equation (eq. V.1.5). The maximum value for Klocation is 1. There is not a minimal value. The advantage above Kappa is that Klocation is independent of the total number of cells in each category.

$$Kloc = \frac{P(A) - P(E)}{P(max) - P(E)} \qquad \text{(eq. V.1.5)}$$

Kquantity is a statistic for disagreement due to quantitative difference. This is more complex than for location, because it is not possible to change quantities of certain categories without changing the locations. It is necessary to correct both for random success and success due to good location specification (eq. V.1.6).

$$Kquantity = \frac{\sum_{i=1}^{c}\left[p_{ii} - Kloc * min\left(\frac{1}{c}, p_{iT}\right)\right] + \frac{Kloc - 1}{c}}{\sum_{i=1}^{c}\left[p_{iT}^{2} + Kloc * \left(p_{iT}^{2} - min\left(\frac{1}{c}, p_{iT}\right)\right)\right] + \frac{Kloc * (1 - c) - 1}{c}} \qquad \text{(eq. V.1.6)}$$

The comparison is not symmetrical. Which means, that comparison of map A to map B yields different results then map B to map A. This means that one map has to be designated as the 'real' or template map. The other map is the 'model' or comparison map (Hagen, 2002b).

After experimenting with the statistics introduced by Pontius, it is recommended not to use the Kquantity statistic, because of the following three reasons (Hagen, 2002b):

1. "The statistic is incomprehensible; it is not possible to give a reasonable explanation to what the formula signifies. For example, it is not clear why the formulation of Kquantity involves Klocation, while the objective is to find a measure for similarity that does not depend on the spatial arrangement.
2. The range of values for the statistic is not the usual Kappa range between –1 and 1; Kquantity can be larger than 1 in cases where Klocation is low and the best overall agreement does not coincide with identical quantitative distributions of the two maps (pers. com. Pontius, 2001).
3. The statistic is not stable; a minor change in the maps can lead to a major change in the statistic. This is a problem, which arises in situations where the denominator has a value close to 0 (pers. com. Pontius 2001)".

Hagen (2002b) proposes an alternative expression for the similarity of the quantitative model that results in the maximal similarity that can be found based upon the total number of cells taken in by each category. This has already been calculated as P(max). P(max) can be put in the context of Kappa and Klocation by scaling it to P(E). The resulting statistic is called Khisto, because it is a statistic that can be calculated directly from the histograms of two maps. Khisto is defined by equation (eq. V.1.7).

$$Khisto = \frac{P(max) - P(E)}{1 - P(E)} \qquad \text{(eq. V.1.7)}$$

The definition of Khisto has the important property that Kappa is now defined as the product of Klocation and Khisto (eq. V.1.8). Klocation is a measure for the similarity of spatial allocation of categories of the two compared maps, and Khisto is a measure for the quantitative similarity of the two compared maps (Hagen, 2002b).

$$K = Khisto * Klocation \qquad \text{(eq. V.1.8)}$$

V.1.3 RESULTS AND DISCUSSION

In Figs.s V.1.2 and V.1.3 is shown the visual map comparison for methods 1, 2 and 3 using respectively, a binary classification which states for each cell whether or not the maps are identical on that location, and class differences.

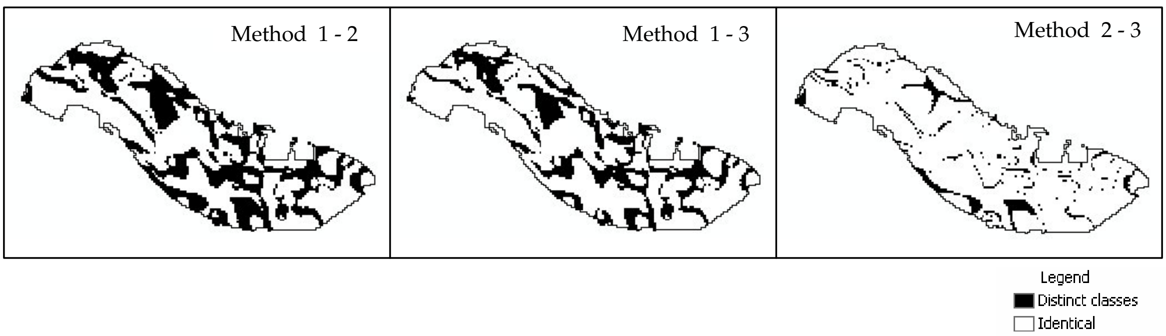

Figure V.1.2 – Map comparison for methods 1, 2 and 3 using Binary classification.

The results of the three different Kappa calculations are presented in Table V.1.3. Analysis of the Kappa values, Figs.s V.1.2 and V.1.3 of the three maps comparison shows an almost perfect agreement (according to Landis and Koch, 1977, see Table V.1.2) between map 2 and 3, confirmed not only for quantity but also for location similarity. This result was expected since method 3 is a refinement of discriminant analysis applied in method 2 using the probabilities of Indicator kriging developed in method 1 (Caeiro *et al.*, 2003). Method 3 is moderately similar to method 1 (Kappa = 0,55) because, although these maps are computed using different multivariate geostatistics, method 3 uses results from method 1. Maps 1 and 2 are the ones with less strength of agreement (Kappa = 0,42) since computed homogenous areas using independent interpolation techniques. Looking at the Klocation value of maps 1-2 (0.51) the differences between these to maps should be more due to spatial location then quantitative dissimilarities (see Table V.1.3).

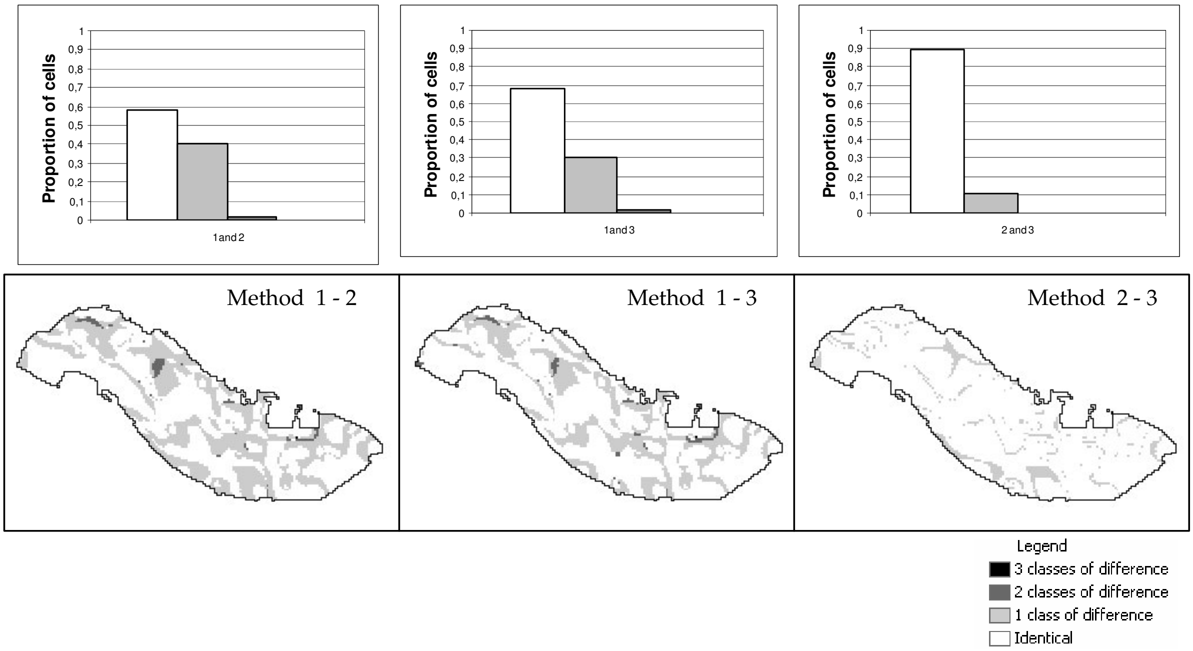

Figure V.1.3 – Map comparison for methods 1, 2 and 3 using class differences and graphs with proportions of cells for each class differences.

Table V.1.3 – The Kappa, Klocation and Khisto results for the 3 map comparison.

Maps	*Kappa* (-1< K<1)	Kloc (max =1)	Khisto (max =1)
1-2	0,42	0.51	0.83
1-3	0,55	0.63	0.87
2-3	0,85	0.95	0.89

Comparison between Map 1-2 in Figs.s V.1.2 and V.1.3 also confirmed this local difference due to less areas of identical classes of classification. This major location difference can also be true for the maps 1-3 comparison since Klocation value are more distance from the maximum value then khisto. In opposition, the small difference between map 2-3 should be due to quantity category values, since Kloc value is almost near maximum similarity. Nevertheless all Klocation values shows agreement substantially greater than agreement expected due to chance (Pontius, 2000). This means that although the tree methods of homogenous areas were computed with different statistical techniques, their results are not completely different.

Despite the good information that Kappa statistics computes, contingency tables reduce overlaid maps to a summary by categories thus losing information about neighborhood, directional and distance relationships, and map pattern (Zaslavsky, 1995). Also, it is as well cell-by-cell comparison in which cells are either identical or non-identical. There are no intermediate similarities. Also, despite Kloc gives an indication of the similarity of the spatial distribution of categories, the statistics does not make a distinction between a category that is dislocated over the distance of one cell, from a cell that is dislocated over the whole map (Hagen, 2002b). Nevertheless Kappa statistics and their variants gives a quick and simple indication of the level of agreement between two maps and guidelines of the source and magnitude of differences between two maps.

V.1.4 CONCLUSION

In this work the advantages of using the Kappa statistics and its new variants to compare maps were demonstrated. The similarity was analyzed not only in terms of location but also in terms of quantity. The Kappa statistics and visual overlay map comparison help us to confirm no gain of precision in using method 3 for homogenous areas delineation and help to find the source of difference between the maps. In future developments fuzzy set theory and fuzzy Kappa statistics will also be used for map comparison. This approach takes both proximity relations and categorical dependencies into account while assessing similarity between two maps (Hagen, 2002a and b).

ACKNOWLEDGMENT

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SADO ESTUARY MANAGEMENT AREAS: HARD VERSUS SOFT CLASSIFICATION MAPS COMPARISON

Caeiro, S., Sousa, S., Gilmore Pontius Jr., R. and Painho, M. (2003)

Proceedings of 5th International Symposium on GIS and Computer Cartography for Coastal Zone Management. 16 – 18 October 2003, GISIG, Genova, Italy, pp.1 – 9.

ABSTRACT

The aim of this work is to assess the difference between three categorical maps of spatially contiguous regions of sediment structure for Sado Estuary in Portugal. These maps were computed for the same purpose but with different spatial statistics. For the map comparison fuzzy classification at different resolutions are used and compared with cell-by-cell and neighborhood hard comparison. These comparison approaches demonstrate that using either single cell, neighborhood hard or soft comparison the three estuarine management areas maps are still similar. Their major differences are mainly due to location disagreement. Advantages of using fuzzy map comparison and evaluation of agreement and disagreement components are discussed.

KEYWORDS: Comparison methods, assessment of map similarity, neighborhood hard or soft comparison, Kappa statistics, components of agreement and disagreement.

V.2.1. INTRODUCTION

In the different Geographical Information Systems (GIS) applications, and particularly in coastal zone management, compare different maps is an essential issue. The accuracy of a comparison procedure based on a more reliable and robust approach could have a marked improvement in the ability to detect a map change. Costal hydrodynamics makes difficult to define sampling grids in exact positions and therefore a single cell-by-cell analysis comparison is less representative. Also in the cell-by-cell agreement between the two maps each cell is crisply classified, since the confusion matrix contains information about only cell-by-cell agreement. The confusion matrix fails to distinguish between a near miss and a far miss. In other words, the confusion matrix records zero agreement when a cell is not classified correctly, even when the correct category is found in the neighbouring cell, or even when the correct category is found nowhere near the cell (Pontius, 2002 and Pontius and Suedmeyer, 2003).

Therefore, a neighborhood cell comparison is more appropriate. Using the neighborhood to compare categorical maps could be computed using a hard or fuzzy classification. Hard classification has the disadvantage of modifying the maps before the comparison. After hardening, there could be a substantial change in the quantity of each category, leading to errors and misleading results. By applying fuzzy classification for the comparison of categorical maps it is possible to obtain a special and gradual analysis of the similarity of two maps (Hagen, 2002). Also, it would be helpful to have on that soft comparison, an analytical technique that allocates the sources of agreement and disagreement indicating if the comparison map is strong or weak.

Within GIS usually the map comparison statistics are used mainly for measuring the goodness-of-fit of simulation land-change models (e.g. Pontius, 2000, Hagen, 2002, Pontius, 2002 and Pontius and Schneider, 2001) and not to evaluate differences between spatial patterns models of regions with very dynamic characteristics like estuaries.

The team has been working on the development of an environmental data management system through sediment quality assessment for the Sado Estuary (EMMSado) in the West Coast of Portugal (Caeiro *et al*., 2002). The units of this management system are spatially contiguous and homogenous regions (management areas). To delineate these management areas three maps were computed using multivariate geostatistical tools. A great agreement of similarities will further support the choice of any of the methods as appropriate for environmental management, and hence the less significance of choosing one of the methods. The aim of this work is to assess the difference between the three maps in which the cells are fuzzy classified, and to separate sources of agreement due to quantity and location. This article comes in the sequence of two other where cell-by-cell comparison and hard neighbourhood classification were computed and results discussed (Sousa *et al.* 2002 and Caiero *et al.,* unpublished). In this work we want also to compare the fuzzy map comparison with this earlier comparison methods.

V.2.2 METHODS

V.2.2.1 Previous work

In order to divide the Sado Estuary in homogenous areas for future environmental management of this ecosystem, geostatistical multivariate techniques were used. Three maps of final homogenous areas were computed from three sediment characterization indicators, using: Map 1) cluster analysis of dissimilarity matrix function of geographical separation followed by indicator kriging of the cluster data, Map 2) discriminant analysis of kriged values of the three sediment attributes, Map 3) combination of methods 1 and 2. (Fig. V.2.1). In each of these categorical maps four organic matter contents categories were computed: 1- for High Organic Load, 2- for Medium High, 3- for Medium, and 4- for Low Organic Load. Results of Map 1 seem to be in better agreement with estuary behavior, assessment of contamination sources and previous work conducted at this site (Caeiro *et al.*, 2003a). For that reason, Map 1 was considered the reference for the comparison between Map 1 and Map 2. For comparison between Map 2 and 3, Map 2 was considered the reference since Map 3 results are from a refinement of Map 2 using data from Map 1. For these same reasons, Map 1 is considered the reference in the comparison between Map 1 and 3.

Visual map overlays were used either for single cell, or neighborhood sizes (3, 5, 7, 9, 11, 13, 15 and 29) using hard data map comparison. The last neighborhood (29) was used to evaluate the sensitivity of this approach. At the finest resolution, each cell is 100-by-100 meters. A two-step process converts the fine-resolution cells to coarse hard-classified cells. For the first step, the size of the coarse cells is determined by aggregating several fine resolution cells. The resolution of the coarse cell is expressed as a multiple of the length of the side of a fine resolution cell. For example, a neighborhood size of 3 means that a 3-by-3 block of fine resolution pixels are aggregated to form one coarse cell. For the second step, a single category is assigned to the coarse cell, based on the majority category among the fine-resolution cells that constitute the coarse cell. Using this neighborhood hard comparison each location is a mode function of the input cells of different neighborhood sizes, instead of a single input cell-by-cell comparison. In both comparisons map algebra and contingency tables were used to obtain the difference between each of the two maps and create a classification of their differences. For quantification of map comparison approaches, Kappa statistics (Kstandard, Klocation to evaluate location errors and Khisto to evaluate quantity errors) and agreement space were used (Sousa *et al.* 2002 and Caeiro *et al.,* unpublished).

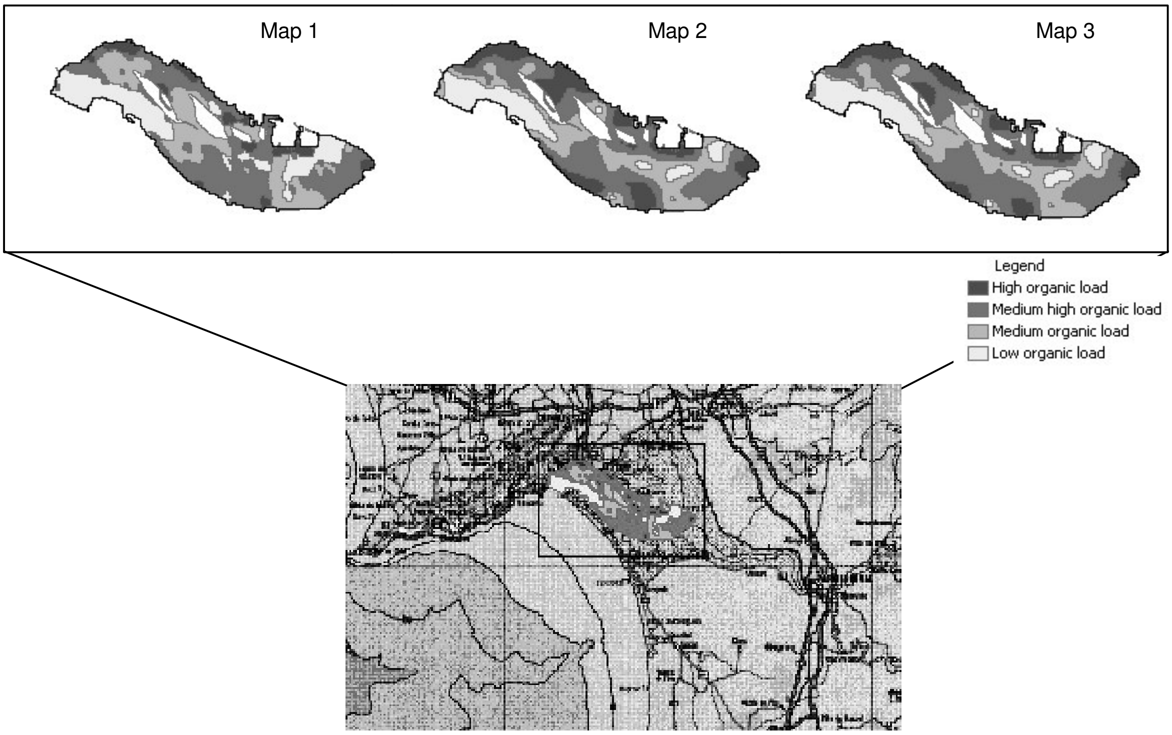


Figure V.2.1 – Study area and maps representing the 3 methods for Sado estuary management area delineation.

V.2.2.2 Fuzzy comparison

For computing fuzzy map comparison the module VALIDATE in Idrisi Kilimanjaro® GIS software was used. The module computes statistics for different resolutions (i.e. length of a fine grid cell size) starting from the resolution of the raw data (finest resolution) to a very coarse resolution. An arithmetic sequence was used to create the aggregating neighboring cells into an increasing coarse grid (from 3 to 29 grid cells). We computed until the grid-cell size of 29 to allow comparing with the previous work.

For maps with one single strata/sub-region VALIDATE computes five especially important numbers that constitute the basis for the components of agreement and disagreement between the reference map and other maps that have increasingly accurate information (from no (n), to medium (m) and perfect information (p)). They are denoted as *N(n)*, *N(m)*, *M(m)* (components of agreement) and , *P(m)* and *P(p)* (components of disagreement). VALIDATE computes these statistics for each resolution. Each cell have partial membership in any of the categories, and the agreement for category *j* in cell *n* is to be minimum of proportion of category *j* in grid cell *n* of Map *M* (*Mn, j*) and proportion of category *j* in grid cell *n* of Map $M^{'}$ (*Mn, j*). Fig. V.2.2 gives the mathematical definition for each expression. For *N(n)*, each cell of the other map is the same and has a membership in each category equal to 1/J. For *N(m)*, each cell of the other map is the same and has a membership in each category equal to the proportion of that category in the comparison map. *M(m)* denotes the proportion correct between the reference map and the comparison map. For *P(m)*, the other map is the comparison map with the locations of the grid swapped anywhere within the map, so as to have the maximum possible agreement with the reference map. For *P(p)*, the agreement between the reference map and the other map that has perfect information of quantity and perfect information of location, therefore the agreement is perfect.

Since the study area is not perfectly square, the aggregation technique will produce coarse resolution cells that are made up of different numbers of fine resolution cells. Therefore, it is important to weigh (*Wn*) each cell according to its importance in the analysis, being *Wn* the number of fine resolution cells that constitute a coarse cell, *n*.

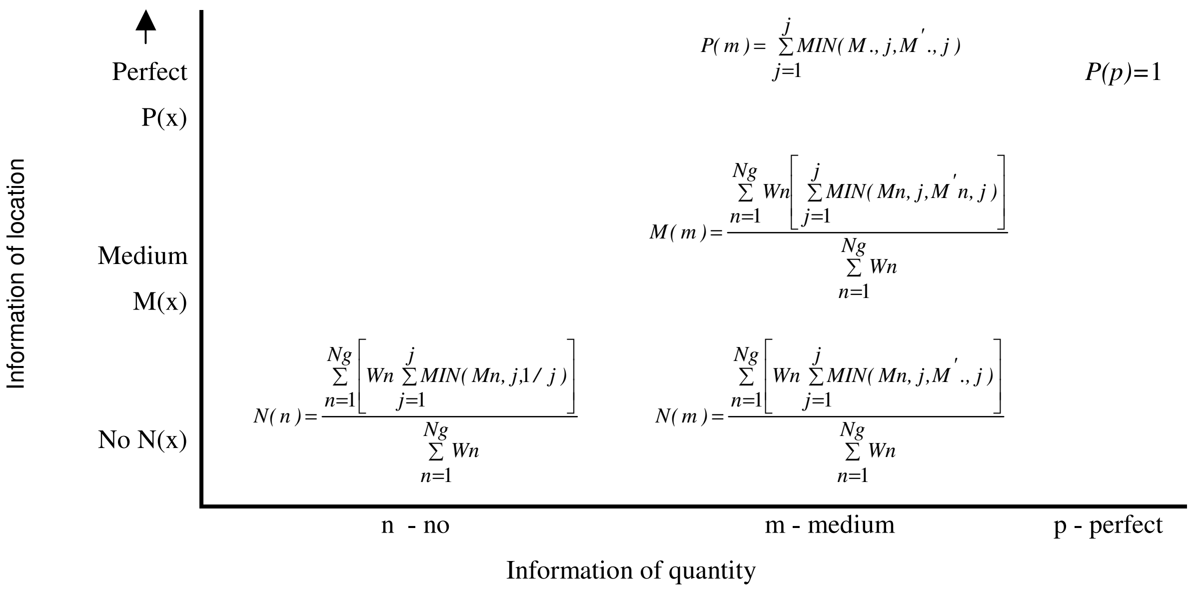


Figure V.2.2 – Mathematical expressions computed by VALIDADE module for map comparison. The expression in the middle column and middle row gives the agreement between reference Map *M* and comparison Map *M'* at resolution *g*. The other four expressions are idealized agreement between *M* and *M'* maps, based on the combination of information available concerning quantity and location. *n* = grid cell index; *j* = category 1 to 4; J = number of categories (4 in our study), *Ng* = number of grid cells in the map at resolution g (from 1 to 29 in our study), *Wn* the number of fine resolution cells that constitute a coarse cell. When a subscript is a dot (.), it means that the term is summed over that subscript (Adapted from Pontius, 2002).

For each resolution the components of agreement are separated into:

1. proportion agreement due to chance = *MIN*[*N(n), N(m), M(m)*];

2. proportion agreement due to quantity = if MIN[*N(n), N(m), M(m)*] = *N(n)*, then MIN[*N(m)*-*N(n)*, *M(m)*-*N(n)*], else 0;
3. proportion agreement due to location = MAX[*M(m) – N(m)*, *0*];
4. proportion disagreement due to location = *P(m) – M(m);*
5. proportion disagreement to quantity = *P(p)-P(m).*

VALIDATE module also computes the Kappa index of agreement and its variants (Pontius, 2000): Kstandard and for location (Klocation), calculated through the following equations:

$$Kstandard = \frac{M(m) - N(m)}{P(p) - N(m)} \qquad \text{(eq. V.2.1)}$$

$$Klocation = \frac{M(m) - N(m)}{P(m) - N(m)} \qquad \text{(eq. V.2.2)}$$

For a more detail and understanding of all these statistics, see (Pontius, 2000, Pontius, 2002 and Pontius and Suedmeyer, 2004).

V.2.3 RESULTS AND DISCUSSION

V.2.3.1 Previous results

Analysis of the three map comparison using only cell-by-cell comparison shows a good agreement between Maps 2 and 3 (Kstandard = 0.85). Maps 1 and 2 are the ones with less agreement since the homogenous areas were computed using independent interpolation techniques. The differences between Maps 1 and 2 and 1 and 3 are mainly due to spatial location (Klocation = 0.51, for comparison between Maps 1 and 2, and Klocation = 0.63 for comparison between Maps 1 and 3) rather to quantity dissimilarities (Khisto = 0.83, for comparison between Maps 1 and 2, and Khisto = 0.87 for comparison between Maps 1 and 3). On the other hand, the small difference between Maps 2 and 3 may be due to the quantity category values, since the Klocation value is close to maximum similarity. Nevertheless all Klocation values show agreement substantially greater than the agreement expected due to chance (Caeiro *et al.*, 2002) (see also Table V.2.1).

Using the hard neighborhood map comparison, the kappa values (Kstandard, Klocation or Khisto) do not vary substantially as cells become coarser, although for grid cell size values higher then 9 the kappa values tend to decrease. Only for neighborhood values that are very high (29 cells, i.e. 2900 m) does the agreement between methods increase substantially (Table V.2.1) (Caeiro *et al.*, Unpublished).

V.2.3.2 Fuzzy comparison

Finest resolution

At the finest resolution the overall proportion correct is 58 %, 68 % and 89 %, for comparison between Maps 1 and 2, 1 and 3 and 2 and 3, respectively. These results are in accordance with Kappa values obtained in the previous studies (see Table V.2.1). A large percent correct is not necessary an important criterion to judge classification schemes because a large portion of percent correct can be attributable to chance (Pontius, 2000). In the case of comparison between Maps 1 and 2, the proportion of disagreement is mainly due to location errors (30 %) and only 12 % is due to quantity disagreement. Also the differences between Maps 1 and 3 are mainly due to location disagreement (23 %) when compared to quantity disagreement (9 %). So, comparing Map 1, with Maps 2 and 3, Map 3 is in more agreement, not only as quantity but also as location (Fig. V.2.3a), V.2.4a), and Table V.2.1).

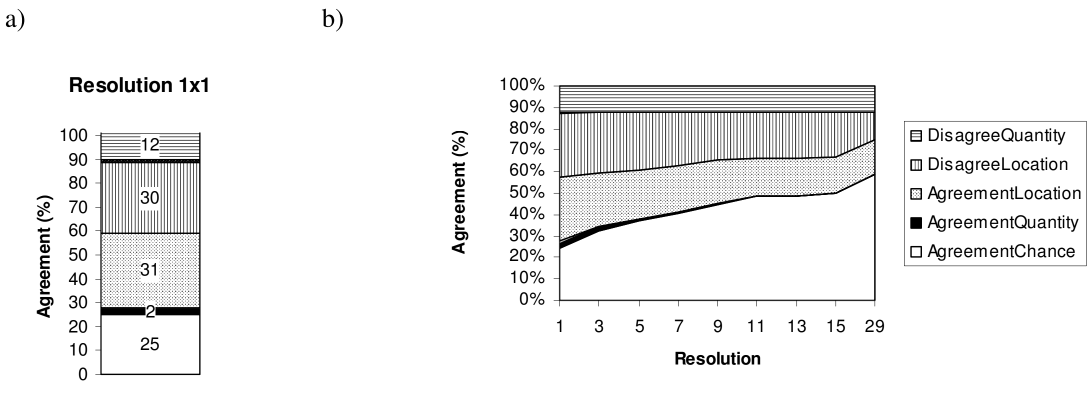


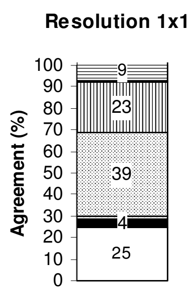
Figure V.2.3 – a) Cumulative percent agreement at fine resolution and b) classification versus resolution for the agreement, between Maps of method 1 and 2.

In contrast, in the more similar Maps (2 and 3) the small differences are due to quantity (8 %), compared to only 3 % due to location disagreement (see Fig. V.2.5a) and Table V.2.1). The refinement of Map 3 (i.e., use of probabilities of Map 1 indicator kriging in discriminate analysis of Map 2) seems to compute mainly small differences in quantity, compared to Map 2.

Multiple resolutions

Figs. V.2.3b), V.2.4b) and V.2.5b) show how percent agreement increases as resolution becomes coarser from 1 to 29 grid cells per side of each coarse grid cell, for all method comparison. At the finest resolution, percent correct due to chance is 25, in all the figures, since there are four categories. As resolution becomes coarser, agreement due to chance tends to increase, agreement due to location decreases, agreement due to quantity doesn't change substantially (or tend to zero in comparison Maps 1 and 2, and 1 and 3), and disagreement due to location decreases. Disagreement due to quantity remains constant since changing the resolution does not change the quantity when the fuzzy aggregation method is used. Both disagreement and agreement due to location decrease as resolution becomes coarser, because location is less important at coarser resolutions.

a)



b)

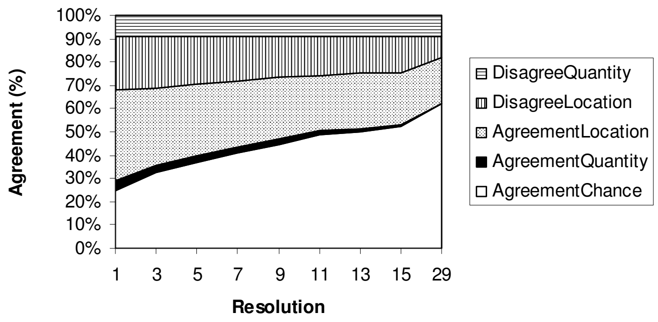
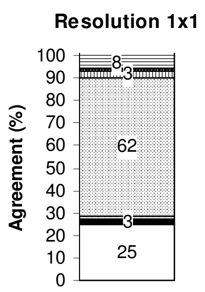


Figure V.2.4 – a) Cumulative percent agreement at fine resolution and b) classification versus resolution for the agreement, between Maps of method 1 and 3.

a)



b)

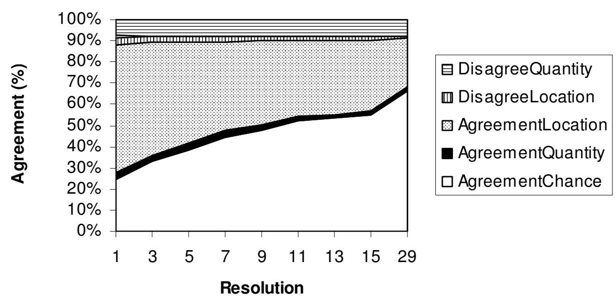


Figure V.2.5 – a) Cumulative percent agreement at fine resolution and b) classification versus resolution for the agreement, between Maps of method 2 and 3.

The percent agreement between Maps 1 and 2 increases from 58 to 75 % as one moves from the finest resolution to the coarsest resolution. On those maps at finest resolution the Kstandard is 0.42, and Klocation is 0.51, as resolution became coarser the Kstandard decreases until the grid cell size reaches 15 and Klocation slightly decreases until grid cell size 7, and increase in the following grid cell (9) and on the coarser one (Figs. V.2.3b), V.2.6 and Table V.2.1).

As resolution becomes coarser, percent agreement between Maps 1 and 3 increases from 68 to 81.7 %, also at the finest resolution the Kstandard is 0.55, and Klocation is 0.63. As resolution becomes coarser Kstandard slightly decreases until grid cell size 15 and Klocation slightly decreases until grid cell size 7, and increases in the coarser grid cells having is higher value (0.68) (Figs. V.2.4b), V.2.6 and Table V.2.1).

Table V.2.1 – *Kstandard* and *Klocation* for the different resolutions and according to hard and soft classification (maximum similarity = 1).

Maps comparison			**1 and 2**	**1 and 3**	**2 and 3**	**1 and 2**	**1 and 3**	**2 and 3**
Kappa				**Kstandard**			**Klocation**	
Resolution	1	Hard or Soft	0.42	0.55	0.85	0.51	0.63	0.95
	3	Hard	0.42	0.55	0.85	0.5	0.63	0.95
		Soft	**0.38**	**0.51**	**0.83**	**0.47**	**0.6**	**0.94**
	5	Hard	0.42	0.55	0.83	0.51	0.64	0.95
		Soft	**0.37**	**0.50**	**0.82**	**0.46**	**0.59**	**0.94**
	7	Hard	0.42	0.56	0.83	0.51	0.64	0.95
		Soft	**0.36**	**0.5**	**0.8**	**0.46**	**0.59**	**0.94**
	9	Hard	0.34	0.47	0.77	0.52	0.58	0.95
		Soft	**0.37**	**0.5**	**0.8**	**0.48**	**0.6**	**0.94**
	11	Hard	0.4	0.54	0.81	0.5	0.63	0.95
		Soft	**0.34**	**0.48**	**0.78**	**0.44**	**0.58**	**0.94**
	13	Hard	0.38	0.53	0.8	0.49	0.62	0.95
		Soft	**0.35**	**0.49**	**0.78**	**0.46**	**0.60**	**0.94**
	15	Hard	0.37	0.53	0.78	0.48	0.64	0.95
		Soft	**0.34**	**0.47**	**0.77**	**0.45**	**0.58**	**0.94**
	29	Hard	0.44	0.56	0.78	0.52	0.74	0.98
		Soft	**0.39**	**0.52**	**0.73**	**0.55**	**0.68**	**0.97**

For both comparisons of Maps 1 and 2 and Maps 1 and 3 the disagreement due to location at resolution 7 is about 90 % the disagreement due to location at resolution 1, indicating that 10 % of the disagreement due to location happens over distances less than 700 m. This grid cell size is similar to the sediment sampling's grid used for computing the maps (750 x 500). This sampling grid was calculated with the principle that there are not important differences in sediment characteristic at distances smaller than the sampling grid (Caeiro, *et al.,* 2003b).

Percent agreement between Maps 2 and 3 increases from 89 to 91.6 % as one move from the finest resolution to the coarsest resolution. The Kstandard decreases as resolution becomes coarser and Klocation is almost constant, only slightly increasing at the coarser resolution.

As well as in hard comparison only for the coarser resolution (29 cells, i.e. 2900 m) does the agreement between methods increase more significantly (see Fig. V.2.6 and Table V.2.1), with the exception of map comparison between Map 2 and 3. This could be due to the less weight of smaller management areas at that resolution.

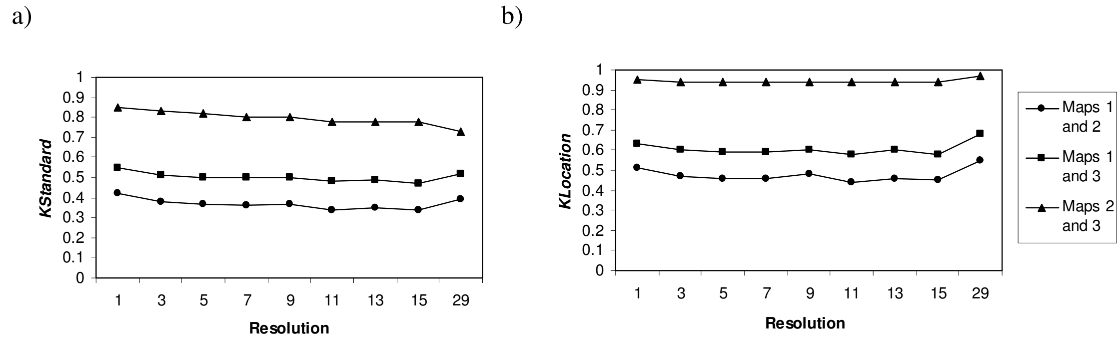


Figure V.2.6 – a) Kstandard and b)Klocation for the different resolutions, calculated using fuzzy classification.

Hard versus soft comparison

Values of KStandard calculated through hard comparison classification show higher variation than the ones calculated through soft classification. This is specially noticed at cell size 9 (see Table V.2.1). As already explained in previous works (Caeiro *et al.*, unpublished), this number of grid cells includes cells of homogenous areas belonging to different organic matter content categories (categories 1 to 4 see Fig. V.2.1) The influence of the hardening step is likely to be the source of this pronounced variation. Similarly, values of Klocation obtained with hard comparison classification are slightly higher then the ones computed through fuzzy classification, because the maps look more similar in terms of location using the hard classification compared to the fuzzy classification.

V.2.4 CONCLUSIONS

In earlier times the map comparison technique was assessed using Kappa index of agreement. However, Kstandard fails to penalize for large quantification error and fails to reward sufficiently for small quantification error. When the quantities of each category in Map *M* is similar to another Map *M'*, then Kappa should indicate so, but Kstandard attributes those correct classifications to chance. Also Kstandard fails to distinguish clearly between quantification error and location error. The classification schemes that attempt to specify accurately both quantity and location are better to evaluate the marginal distributions in spatial models (Pontius, 2000). The new methods presented here of accuracy assessment allows to budget the component of agreement and disagreement between any two maps that show a categorical variable, not only at raw map resolution but also at multiple resolutions using fuzzy classification (Pontius and Suedmeyer, 2003). These techniques compare the maps in terms of quantity and location.

In this work we have shown a complementary application of these comparison techniques, which are usually used for remote sensing, simulation modeling and land change analysis. Our application has been to evaluate the differences between three spatial models of estuarine sediment management areas. The different comparison approaches demonstrated that using either single cell, neighborhood hard or soft comparison the three estuarine management areas maps are still similar, being the differences mainly due to location disagreement. All the results reinforce the robustness of the method for management area calculation. Moreover, support the choice of any of the methods as appropriate for environmental management, and hence moderate the significance of choosing the map resulting from method 1.

Nevertheless there are advantages in using fuzzy classification and budget assessment of component of agreement and disagreement. Fuzzy agreement maps compared with earlier works of hard comparison contains more information and gives a more easy and realistic interpretation of the dataset. As explained in the introduction the hard classification changes the maps leading to misleading results.

ACKNOWLEDGMENTS

The research was funded by the Portuguese Science and Technology Foundation and POCTI (Research Project nº POCTI/BSE 35137/99) and financed by FEDER. Sandra Caeiro holds a PRODEP grant.

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ANNEX VI –APPLICATION OF THE DPSIR MODEL TO THE SADO ESTUARY IN A GIS CONTEXT – SOCIAL AND ECONOMICAL PRESSURE: SUPPORT INFORMATION

APPLICATION OF THE DPSIR MODEL TO THE SADO ESTUARY IN A GIS CONTEXT – SOCIAL AND ECONOMICAL PRESSURE: SUPPORT INFORMATION

Caeiro, S., Mourão, I., Costa, M. H., Painho, M., Ramos, T. B., Sousa, S. (2004)

Topen, F., Prastacos (Ed.) *Proceedings of 7th AGILE Conference on Geographic Information Science* Greece, Heraklion, 29 April - 1 May of 2004, pp. 391 – 402.

Table VI.1 - Urban use and population density in each village (in the year 2002).

Village	**Area (km^2)**	**% Setúbal sub watershed Area**	**Population density (inhab.km^{-2})**
Gambia-Pontes-Alto da Guerra	0.68	0.30	125
Marateca	0.01	0.00	27
Palmela	1.50	0.66	214
Sado	1.20	0.53	142
São Loureço	0.06	0.03	178
São Simão	0.02	0.01	214
Setúbal (Nossa Senhora da Anunciada)	1.41	0.62	587
Setúbal (Santa Maria da Graça)	1.00	0.44	7630
Setúbal (São Julião)	1.26	0.56	4107
Setúbal (São Sebastião)	3.16	1.40	2511
Total urban area in the sub-basin (km^2)	**10.28**	**4.55**	**15724**

Source: IGEO, 2003 and INE, 2003.

Table VI.2 - Annual load estimations per village and annual non-point source pollution loads.

Village	**BOD (t.y^{-1})**	**N (t.y^{-1})**	**P (t.y^{-1})**	**TSS (t.y^{-1})**
Palmela	317.64	53.18	6.41	708.82
Setúbal (Nossa Sr.ª Anunciada)	317.17	53.10	6.40	707.77
Setúbal (Santa Maria da Graça	105.25	17.62	2.12	234.87
Setúbal (São Julião)	336.45	56.32	6.79	750.78
São Lourenco	167.28	28.00	3.38	373.28
Setúbal (São Sebastião)	1040.96	174.27	21.01	2322.89
São Simao	90.63	15.17	1.83	202.23
Gambia-Pontes-Alto da Guerra	80.34	13.45	1.62	179.27
Sado	107.56	18.01	2.17	240.01
Marateca	70.68	11.83	1.43	157.72
Total per village	**2633.97**	**440.95**	**53.17**	**5877.65**
Annual non source pollution loads (INAG, 2001)	**453.73 (8402435 inhab-eq.y^{-1})**	**45010.00 (4978979535 inhab-eq.y^{-1})**	**1295.13 (1188192202 inhab-eq.y^{-1})**	**2771.50 (23000000 inhab-eq.y^{-1})**

Table VI.3 - Groups of Salt-pans and aquaculture and their areas in the Sado Estuary. (Setúbal and Alcacer do Sal municipalities.

	Salt-pan	**Aquaculture**
Group	**Area (km^2)**	**Area (km^2)**
Faralhão	0.40	0.89
Gambia	0.61	1.10
Mitrena	0.22	0.32
Monte de Cabras	0.95	0.06
Mouriscas	0.52	0.12
Pinheiro Torto	0.19	0.09
Praias do Sado	0.97	0.36
Sachola	0.00	1.19
Vaia	0.70	0.47
Vale de Judeus	0.21	0.18
Batalha	1.00	0.00
Bocas de Palma	0.80	0.03
Cachopos	0.00	0.20
Comporta	0.08	0.00
Enxarroqueira	0.34	0.03
Faias	0.13	0.08
Monte da Pedra	0.58	0.00
Torrinha e Casas Novas	0.68	0.00
Total area (km^2)	**8.36**	**5.12**

Source: Dias, 1994.

TableVI.4 - Annual number of ships that discharged in the fishing docks.

Fishing	Ships.y^{-1}				
dock	1998	1999	2000	2001	2002
Setúbal	355	318	318	318	277
Gâmbia	77	77	77	77	78
Carrasqueira	48	43	43	43	50
Total	**480**	**438**	**438**	**438**	**405**

Source: DocaPesca (MAP).

Table VI.5 – Total values of annual fish fresh-weight discharged in Sado estuary docks.

Fishing	**Captured fish fresh weight - t.y^{-1} (t.y^{-1}.boat^{-1})**				
dock	**1998**	**1999**	**2000**	**2001**	**2002**
Setúbal	2474157 (6969)	3015106 (9481)	3466322 (10900)	3124695 (9826)	2575168 (9297)
Gâmbia	68114 (885)	38832 (504)	46523 (604)	86145 (1119)	183330 (2350)
Carrasqueira	69917 (1457)	52731 (1226)	66691 (1551)	70775 (1646)	86529 (1731)
Total	**2612188 (9311)**	**3106669 (11211)**	**3579536 (13055)**	**3281615 (12591)**	**2845027 (13378)**

Source: DocaPesca (MAP).

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ANNEX VII – ASSESSING SEDIMENT HEAVY METALS CONTAMINATION IN THE SADO ESTUARY: SUPPORT INFORMATION

ASSESSING SEDIMENT HEAVY METALS CONTAMINATION IN THE SADO ESTUARY: AN INDEX ANALYSIS APPROACH

Caeiro, S., Costa, M. H., Ramos, T. B., Fernandes, F., Silveira, N., Coimbra, A., Medeiros, G. and Painho, M. (2003).

Abstract proceedings of CICTA 2003 – 5th Iberian and 2nd Iberoamerican Congress of Environmental Contamination and Toxicology. Environmental Problems in an Iberoamerican Context. 22 – 24 September 2003, Porto, Portugal, pp.147.

(submitted to *Ecological Indicators*).

Table VII.1 – Physical and chemical data in the 78 sampling locations.

Nº Am	PIN	DC	PLI	SQGQ	MPI	I	NI	MSPI	Cd* (ugg^{-1})	Pb* (ugg^{-1})	Zn* (ugg^{-1})	Cu* (ugg^{-1})	As* (ugg^{-1})	Cr* (ugg^{-1})	Hg* (ugg^{-1})	TOM* (%)	FF (%)	Eh (mV)	Al* (ugg^{-1})
1	3	12.62	0.45	0.66	2.01E+08	13.92	9.41	100.00	5.80	64.00	206.00	59.00	22.00	33.00	0.43	10.70	55.98	-391.00	2.25
2	2	6.29	2.22	0.33	1.61E+06	6.79	4.60	73.66	2.80	24.00	98.00	30.00	15.00	20.00	0.19	6.02	26.45	-298.30	1.13
4	1	2.85	4.98	0.15	3.12E+03	3.08	2.35	32.95	1.30	28.00	34.00	7.00	7.20	5.00	0.07	5.23	14.25	-189.10	0.25
8	1	1.53	8.19	0.07	1.73E+00	0.88	0.85	8.19	0.90	2.00	4.00	4.00	3.00	2.00	0.07	0.46	0.31	83.10	0.02
10	1	0.96	9.29	0.05	1.80E-01	0.65	0.68	5.20	0.30	3.50	7.40	1.00	4.50	0.60	0.06	0.84	0.37	93.70	0.01
11	1	0.83	9.60	0.04	9.95E-02	0.62	0.64	6.49	0.20	3.60	6.40	1.00	3.60	0.60	0.07	0.66	0.35	108.50	0.02
14	2	7.52	1.78	0.38	3.32E+06	7.49	5.20	84.39	3.50	17.00	110.00	31.00	21.00	26.00	0.21	5.74	33.83	-102.00	1.93
16	1	2.46	6.13	0.12	1.12E+03	2.25	1.66	29.65	1.10	6.20	32.00	10.00	7.50	6.00	0.08	2.32	8.86	-145.00	0.40
17	2	8.83	1.38	0.47	2.00E+07	9.60	6.61	94.75	3.20	26.00	149.00	46.00	21.00	26.00	0.45	6.85	39.40	-245.00	1.88
19	2	8.71	1.29	0.44	1.12E+07	8.95	6.02	94.75	3.90	21.00	130.00	48.00	21.00	26.00	0.28	6.93	34.85	-275.00	1.64
21	1	2.32	6.09	0.12	9.49E+02	2.29	1.63	23.86	1.00	5.10	34.00	9.00	7.60	8.00	0.07	2.86	12.50	-109.00	0.57
23	2	2.97	6.79	0.15	3.02E+02	1.85	1.89	20.86	1.00	3.50	24.00	5.00	21.00	4.00	0.06	1.29	6.10	-66.00	0.30
24	1	2.10	7.54	0.09	1.27E+01	1.12	1.16	11.72	1.10	2.00	9.00	4.00	8.00	2.00	0.07	0.68	0.45	137.00	0.01
25	1	2.31	8.26	0.12	5.14E+00	1.31	1.54	13.56	0.40	3.40	2.10	10.00	21.00	1.00	0.06	1.04	0.56	101.00	0.03
26	1	1.21	9.37	0.06	2.82E-01	0.71	0.86	7.92	0.30	3.60	3.30	1.00	7.90	1.00	0.07	0.57	0.44	104.00	0.03
31	1	0.96	8.70	0.04	3.92E-01	0.75	0.64	4.00	0.50	3.30	6.30	2.00	1.10	2.00	0.06	1.34	2.86	-137.00	0.07
32	1	1.12	8.63	0.05	1.95E+00	0.85	0.75	4.00	0.50	3.10	7.90	3.00	3.10	2.00	0.06	1.15	2.67	-160.00	0.10

Table VII.1 – Physical and chemical data in the 78 sampling locations (cont.).

Nº Am	PIN	DC	PLI	SQGQ	MPI	I	NI	MSPI	Cd* (ugg^{-1})	Pb* (ugg^{-1})	Zn* (ugg^{-1})	Cu* (ugg^{-1})	As* (ugg^{-1})	Cr* (ugg^{-1})	Hg* (ugg^{-1})	TOM* (%)	FF (%)	Eh (mV)	Al* (ugg^{-1})
33	1	2.80	5.74	0.17	8.61E+03	3.79	2.56	46.63	0.20	8.90	56.00	21.00	12.00	12.00	0.20	3.56	14.78	-239.00	0.98
34	3	19.95	0.14	1.03	3.69E+09	21.26	13.85	100.00	8.00	36.00	272.00	149.00	54.00	63.00	0.65	3.35	94.75	-324.00	5.18
35	3	14.20	0.38	0.73	3.14E+08	14.80	9.68	100.00	6.00	28.00	213.00	98.00	33.00	38.00	0.50	8.37	49.29	-299.00	2.98
36	2	4.49	3.25	0.23	8.93E+04	4.53	3.06	68.92	2.00	8.90	67.00	24.00	13.00	14.00	0.12	6.53	30.33	-202.00	1.07
37	2	4.52	4.47	0.23	5.50E+04	3.96	3.23	59.47	1.60	9.40	56.00	15.00	9.40	9.00	0.36	2.80	16.21	-166.00	0.62
39	2	6.32	2.38	0.33	1.67E+06	6.97	4.53	79.07	2.50	16.00	104.00	42.00	16.00	19.00	0.22	4.24	27.25	-192.00	1.34
40	3	16.31	0.24	0.85	1.13E+09	17.50	11.67	100.00	6.50	35.00	273.00	92.00	41.00	52.00	0.65	9.96	92.21	-294.00	3.83
43	3	18.70	0.07	1.08	4.08E+09	25.97	14.10	100.00	6.40	69.00	507.00	191.00	37.00	44.00	0.41	8.50	71.95	-149.00	3.30
52	1	2.76	5.98	0.14	1.17E+03	2.47	1.81	29.35	1.20	5.00	57.00	6.00	10.00	5.00	0.08	1.24	6.25	-190.00	0.30
53	2	4.22	3.93	0.21	3.72E+04	4.32	2.85	60.35	2.10	8.30	79.00	15.00	12.00	15.00	0.07	1.97	10.79	-248.00	1.03
55	1	2.52	6.38	0.12	2.23E+02	2.02	1.51	16.12	1.30	5.00	49.00	5.00	7.00	2.00	0.07	0.52	1.42	-65.00	0.10
56	2	3.61	5.23	0.18	1.99E+04	3.44	2.55	51.14	1.50	8.40	52.00	13.00	9.10	10.00	0.18	0.89	6.95	-175.10	0.71
57	2	4.36	3.86	0.22	6.05E+04	4.28	2.97	68.92	2.20	13.00	69.00	15.00	11.00	13.00	0.10	2.49	11.08	74.00	0.35
58	2	4.94	3.18	0.25	1.81E+05	4.94	3.40	68.92	2.30	11.00	74.00	22.00	12.00	16.00	0.16	4.64	20.84	-399.00	1.21
59	1	2.22	6.58	0.10	1.54E+02	1.69	1.33	24.13	1.30	5.30	20.00	7.00	4.00	4.00	0.07	1.45	4.18	-145.00	0.24
60	1	1.28	8.19	0.06	5.38E+00	1.00	0.83	5.30	0.60	3.30	12.00	4.00	3.30	2.00	0.06	1.44	4.86	-224.00	0.15
61	2	4.28	2.78	0.21	5.85E+04	3.94	2.98	59.46	1.80	10.00	56.00	16.00	11.00	11.00	0.21	13.36	13.68	-164.00	0.76
63	1	1.17	8.06	0.06	6.24E+00	1.08	0.86	8.04	0.40	3.70	19.00	3.00	3.70	2.00	0.07	2.44	12.41	-125.00	0.12
65	1	2.81	5.08	0.14	4.45E+03	2.94	2.00	40.16	1.20	7.00	42.00	14.00	9.00	10.00	0.07	4.39	19.31	-175.00	0.68
68	2	10.30	1.38	0.53	2.76E+07	9.54	7.53	100.00	3.70	23.00	131.00	34.00	26.00	28.00	0.70	5.59	29.08	-278.00	1.36
70	2	3.01	5.40	0.15	4.76E+03	2.88	2.05	36.00	1.40	8.00	47.00	11.00	9.00	8.00	0.08	2.08	10.49	-177.00	0.40
74	1	1.50	8.34	0.07	7.78E+00	1.02	0.97	4.00	0.60	3.00	12.00	3.00	7.00	2.00	0.06	0.88	0.72	50.50	0.25
75	1	1.64	7.42	0.08	2.46E+01	1.39	1.05	13.68	0.80	4.00	28.00	4.00	3.00	2.00	0.08	1.47	2.03	-168.20	0.07
76	2	2.89	5.83	0.14	1.47E+03	2.51	1.85	26.68	1.50	8.00	51.00	6.00	8.00	5.00	0.07	0.65	1.62	55.00	0.22

Table VII.1 – Physical and chemical data in the 78 sampling locations (cont.).

Nº Am	PIN	DC	PLI	SQGQ	MPI	I	NI	MSPI	Cd* (ugg^{-1})	Pb* (ugg^{-1})	Zn* (ugg^{-1})	Cu* (ugg^{-1})	As* (ugg^{-1})	Cr* (ugg^{-1})	Hg* (ugg^{-1})	TOM* (%)	FF (%)	Eh (mV)	Al* (ugg^{-1})
80	2	3.41	4.27	0.18	1.07E+04	3.70	2.29	40.35	1.60	8.00	82.00	16.00	8.00	8.00	0.07	3.59	15.01	-126.00	1.62
82	1	2.35	6.39	0.12	4.20E+02	1.96	1.55	23.37	1.00	4.00	34.00	6.00	9.00	5.00	0.08	2.48	12.04	-27.00	0.25
85	1	1.33	8.45	0.07	4.45E+00	1.16	0.94	6.60	0.40	3.50	29.00	2.00	6.40	1.00	0.06	0.72	1.00	114.50	0.03
86	1	2.33	6.06	0.14	9.30E+02	3.19	2.07	26.56	0.70	19.00	85.00	3.00	8.00	4.00	0.06	1.42	4.97	-192.00	0.16
90	2	8.82	1.43	0.46	1.32E+07	8.71	6.51	100.00	3.30	23.00	131.00	31.00	23.00	26.00	0.50	8.68	48.68	-225.00	12.90
93	2	5.31	5.97	0.27	1.67E+03	2.81	3.59	23.36	0.80	5.00	28.00	6.00	58.00	5.00	0.06	2.21	7.60	-40.00	0.22
95	1	1.60	6.84	0.09	5.16E+01	2.07	1.13	11.98	0.60	4.00	57.00	11.00	2.00	2.00	0.06	1.63	7.52	-126.00	0.09
98	1	2.74	5.42	0.14	2.61E+03	2.88	1.92	36.69	1.20	6.00	58.00	9.00	9.00	9.00	0.06	2.66	13.29	-127.10	0.49
102	3	12.40	0.53	0.60	6.85E+06	11.33	7.78	78.80	6.30	2.00	199.00	43.00	38.00	45.00	0.26	9.09	81.43	-317.00	1.76
104	2	3.57	4.50	0.18	1.51E+04	3.55	2.46	51.13	1.60	8.00	65.00	12.00	12.00	11.00	0.08	3.35	15.69	-180.40	0.70
105	2	3.22	4.53	0.17	7.08E+03	3.36	2.23	36.69	1.50	7.00	65.00	11.00	10.00	11.00	0.06	4.18	11.35	-149.00	0.59
108	1	2.40	6.08	0.12	1.03E+03	2.34	1.65	27.05	1.10	6.00	40.00	8.00	7.00	7.00	0.07	2.21	8.74	-60.00	0.35
111	1	1.79	7.63	0.09	5.73E+01	1.38	1.22	18.51	0.70	4.00	16.00	4.00	8.00	4.00	0.07	1.62	4.52	176.10	0.11
113	2	2.75	5.53	0.14	2.03E+03	2.58	1.83	27.05	1.40	7.00	41.00	9.00	7.00	8.00	0.07	2.45	6.88	-134.20	0.45
116	1	1.51	8.30	0.07	8.42E+00	1.03	0.97	4.00	0.60	3.00	13.00	3.00	7.00	2.00	0.06	0.95	0.63	144.30	0.02
117	1	1.98	7.64	0.10	4.74E+01	1.34	1.26	17.90	0.80	4.00	18.00	4.00	9.00	2.00	0.08	1.07	1.29	45.00	0.06
118	1	1.55	8.14	0.08	1.85E+01	1.21	1.04	6.71	0.60	3.00	19.00	3.00	7.00	3.00	0.06	0.85	1.28	2.00	0.04
119	2	2.94	5.38	0.15	3.03E+03	2.71	1.97	36.00	1.40	7.00	47.00	8.00	9.00	8.00	0.08	2.65	8.17	-218.00	0.41
125	3	10.92	0.74	0.54	2.86E+07	10.45	7.24	100.00	5.60	22.00	162.00	39.00	29.00	37.00	0.24	8.38	62.61	-302.30	1.34
128	1	3.12	5.65	0.16	4.00E+03	2.78	2.29	29.44	1.00	5.00	37.00	10.00	7.00	8.00	0.27	3.43	29.47	-220.20	0.11
131	2	3.75	4.40	0.19	2.32E+04	3.80	2.60	64.56	1.80	9.00	58.00	14.00	11.00	14.00	0.08	2.60	13.75	-243.90	0.72
132	1	1.33	8.45	0.06	1.34E+00	0.84	0.79	8.19	0.70	2.00	4.00	4.00	3.00	2.00	0.07	0.78	0.61	115.00	0.03

Table VII.1 – Physical and chemical data in the 78 sampling locations (cont.).

Nº Am	PIN	DC	PLI	SQGQ	MPI	I	NI	MSPI	Cd* (ugg^{-1})	Pb* (ugg^{-1})	Zn* (ugg^{-1})	Cu* (ugg^{-1})	As* (ugg^{-1})	Cr* (ugg^{-1})	Hg* (ugg^{-1})	TOM* (%)	FF (%)	Eh (mV)	Al* (ugg^{-1})
136	2	4.01	4.24	0.20	3.27E+04	3.91	2.77	59.26	1.80	10.00	70.00	12.00	14.00	12.00	0.09	2.88	9.69	-158.20	0.03
138	1	1.18	8.40	0.06	2.10E+00	0.96	0.74	5.24	0.60	2.00	17.00	3.00	2.00	2.00	0.06	0.78	0.77	100.00	0.02
139	3	14.68	0.25	0.79	7.35E+08	17.46	10.86	100.00	5.90	48.00	295.00	94.00	39.00	48.00	0.35	10.80	87.09	-256.80	3.70
147	1	1.73	7.29	0.08	4.34E+01	1.40	1.13	12.17	0.80	3.00	22.00	4.00	6.00	4.00	0.06	2.01	6.59	-103.20	0.21
148	1	1.53	8.20	0.08	8.64E+00	1.11	0.98	5.24	0.60	2.00	20.00	3.00	7.00	2.00	0.06	0.81	0.95	50.10	0.03
149	1	1.53	8.09	0.08	1.46E+01	1.14	1.02	5.30	0.60	3.00	15.00	3.00	7.00	3.00	0.06	1.27	2.49	39.90	0.06
150	3	15.52	0.26	0.78	4.55E+08	15.40	10.55	100.00	7.40	33.00	219.00	70.00	45.00	54.00	0.35	11.10	96.11	-268.70	1.91
151	1	1.66	7.66	0.08	1.56E+01	1.15	1.03	6.74	0.80	3.00	14.00	3.00	6.00	3.00	0.06	1.67	3.23	44.70	0.04
153	2	5.25	2.61	0.25	3.72E+04	5.09	3.31	60.78	3.00	10.00	86.00	20.00	14.00	18.00	0.02	5.42	26.22	-210.30	0.78
156	2	3.75	4.16	0.19	1.79E+04	3.83	2.59	51.64	1.70	7.00	74.00	12.00	13.00	13.00	0.07	3.83	19.68	-94.30	0.84
157	3	13.26	0.42	0.67	1.42E+08	13.54	9.18	100.00	6.20	24.00	221.00	49.00	41.00	52.00	0.29	9.56	90.51	-198.60	2.60
800	1	1.45	8.08	0.07	2.16E+00	0.85	0.90	4.00	0.60	2.00	5.00	3.00	7.00	2.00	0.06	2.24	6.50	-101.40	0.05
1110	1	1.50	8.31	0.07	7.78E+00	1.02	0.97	4.00	0.60	3.00	12.00	3.00	7.00	2.00	0.06	0.99	1.86	164.10	0.08
1111	2	3.27	4.93	0.16	4.25E+03	2.79	2.09	47.10	1.70	6.00	40.00	10.00	9.00	9.00	0.09	3.24	14.52	-213.10	0.48
1240	1	2.55	6.36	0.12	5.99E+02	2.07	1.62	21.12	1.30	5.00	32.00	6.00	8.00	6.00	0.07	1.03	3.78	-9.00	0.33

*** -** replicates with standard deviations lower than 20 %.

ANNEX VIII – BENTHIC BIOTOPE INDEX DEVELOPMENT FOR THE SADO ESTUARY, PORTUGAL: SUPPORT INFORMATION

BENTHIC BIOTOPE INDEX DEVELOPMENT FOR THE SADO ESTUARY, PORTUGAL: SUPPORT INFORMATION

Caeiro, S., Costa, M. H., Goovaerts, P. and Martins, F.

submitted to *Marine Environmental Research*

Table VIII.1 –Physical, chemical, hydrodynamic data and Biotic index results in the 77 sampling locations.

Locations	% FF	% sand	% gravel	% TOM	Shear stress (Nm^{-2})	Flow (m^2s^{-1})	Velocity (ms^{-1})	Depth (m)	Bi_{bio}
1	56.0	34.8	9.2	10.7	1.6	0.9	0.16	5.9	4.6
2	26.5	59.1	14.5	6.0	1.0	1.1	0.13	8.3	3.4
4	14.3	72.4	13.4	5.2	3.0	7.4	0.45	16.6	1.0
7	63.8	25.7	10.6	7.1	1.3	7.2	0.27	26.6	4.7
10	0.4	87.0	12.6	0.8	3.0	6.6	0.51	12.9	1.2
11	0.4	92.5	7.2	0.7	3.9	10.7	0.55	19.3	1.0
14	33.8	58.3	7.8	5.7	3.2	10.6	0.46	22.8	1.0
16	8.9	74.0	17.1	2.3	2.0	5.0	0.37	13.6	2.4
17	39.4	53.6	7.0	6.9	1.7	4.2	0.37	11.4	3.5
19	34.9	53.6	11.6	6.9	1.2	4.8	0.30	16.1	3.4
21	12.5	78.9	8.6	2.9	0.7	1.7	0.23	7.2	3.2
23	6.1	90.4	3.5	1.3	1.1	3.2	0.27	11.6	2.7
24	0.5	86.2	13.3	0.7	1.3	4.9	0.28	17.7	2.3
25	0.6	96.3	3.1	1.0	1.3	2.1	0.26	7.7	2.7
26	0.4	98.0	1.6	0.6	1.6	1.8	0.30	5.9	2.8
31	2.9	92.5	4.7	1.3	2.4	2.8	0.42	6.7	2.7
32	2.7	89.6	7.7	1.2	1.8	3.0	0.38	7.9	2.7
33	14.8	67.4	17.9	3.6	1.4	4.4	0.29	15.1	2.6
34	94.7	4.7	0.6	3.4	1.2	2.2	0.26	8.3	5.0
35	49.3	48.0	2.7	8.4	1.0	2.8	0.28	9.9	4.3
36	30.3	30.7	39.0	6.5	1.1	3.0	0.29	10.3	3.6
37	16.2	71.0	12.7	2.8	3.4	1.6	0.22	7.3	1.0
39	27.2	68.2	4.6	4.2	1.5	2.9	0.29	9.8	3.1
40	92.2	7.8	0.0	10.0	1.6	1.8	0.34	5.2	5.0
43	72.0	27.2	0.8	8.5	0.7	1.2	0.15	7.7	4.9
52	6.3	91.8	2.0	1.2	2.9	2.3	0.46	5.0	2.6
53	10.8	85.7	3.5	2.0	1.5	1.1	0.30	3.6	3.0
55	1.4	94.2	4.3	0.5	1.4	13.0	1.07	11.9	3.0
56	7.0	86.8	6.3	0.9	2.5	5.0	0.42	11.9	2.1
57	11.1	68.0	21.0	2.5	1.7	4.2	0.37	11.5	2.7
58	20.8	67.5	11.7	4.6	1.8	3.2	0.35	8.9	3.0
59	4.2	85.5	10.3	1.4	1.6	2.1	0.32	6.5	2.8
60	4.9	87.3	7.9	1.4	1.9	0.9	0.33	2.8	2.9
61	13.7	81.1	5.3	13.4	2.1	0.9	0.37	2.4	3.6
63	12.4	81.4	6.2	2.4	2.0	2.3	0.38	5.9	2.9
65	19.3	73.8	6.8	4.4	1.1	4.5	0.28	16.1	2.8

Table VIII.1 – Biological, physical/hydrodynamic data in the 77 sampling locations (cont.).

Locations	% FF	% sand	% gravel	% TOM	Shear stress (Nm^{-2})	Flow (m^2s^{-1})	Velocity (ms^{-1})	Depth (m)	Bi_{bio}
68	29.1	58.8	12.1	5.6	0.9	1.4	0.20	6.6	3.6
70	10.5	85.9	3.6	2.1	1.4	0.6	0.31	2.0	3.1
74	0.7	92.3	7.0	0.9	1.1	1.7	0.23	7.4	2.8
75	2.0	94.1	3.9	1.5	3.0	4.0	0.48	8.2	1.6
76	1.6	94.4	4.0	0.6	1.1	2.0	0.25	7.9	2.8
80	15.0	72.0	13.0	3.6	1.5	2.7	0.34	7.9	3.0
82	12.0	83.5	4.5	2.5	1.4	1.9	0.27	6.9	2.9
85	1.0	96.0	3.0	0.7	2.2	3.5	0.40	8.8	2.6
86	5.0	89.8	5.2	1.4	2.0	4.2	0.37	11.3	2.5
90	48.7	43.9	7.4	8.7	1.3	1.7	0.30	5.7	4.2
93	7.6	84.6	7.8	2.2	1.8	1.5	0.37	4.0	2.9
95	7.5	81.1	11.4	1.6	1.9	2.1	0.32	6.6	2.8
98	13.3	78.0	8.7	2.7	1.9	3.9	0.37	10.4	2.7
102	81.4	18.4	0.1	9.1	2.1	0.9	0.32	2.5	4.9
104	15.7	66.3	18.0	3.3	0.9	2.3	0.26	8.8	3.2
105	11.4	77.9	10.8	4.2	0.9	2.7	0.24	10.9	3.0
108	8.7	82.6	8.6	2.2	1.8	4.4	0.39	11.3	2.6
111	4.5	82.0	13.5	1.6	2.1	3.2	0.36	8.8	2.6
113	6.9	89.3	3.9	2.4	2.1	3.4	0.36	9.4	2.5
116	0.6	93.2	6.2	0.9	1.2	5.7	0.29	19.1	2.2
117	1.3	91.9	6.8	1.1	2.0	4.0	0.29	13.8	1.6
118	1.3	89.9	8.8	0.8	2.2	6.4	0.39	16.2	1.7
119	8.2	80.2	11.6	2.6	1.7	4.6	0.37	12.6	2.5
125	62.6	36.6	0.7	8.4	1.3	1.4	0.26	5.0	4.7
128	29.5	68.7	1.8	3.4	2.0	1.4	0.37	3.7	3.1
131	13.8	72.3	14.0	2.6	0.8	1.6	0.25	6.1	3.2
132	0.6	98.9	0.5	0.8	1.4	2.0	0.24	8.3	2.7
136	9.7	85.4	4.9	2.9	2.1	3.9	0.37	10.4	2.6
138	0.8	96.4	2.9	0.8	2.1	0.9	0.34	2.7	2.9
139	87.1	12.9	0.0	10.8	1.4	3.4	0.32	10.6	5.0
147	6.6	85.9	7.5	2.0	2.4	1.4	0.43	3.1	2.9
148	1.0	88.1	10.9	0.8	2.4	2.4	0.39	6.3	2.6
149	2.5	90.3	7.3	1.3	2.5	1.5	0.40	3.7	2.8
150	96.1	3.9	0.0	11.1	2.3	1.9	0.35	5.5	5.0
151	3.2	76.6	20.2	1.7	2.3	1.6	0.37	4.1	2.8
153	26.2	58.6	15.2	5.4	1.1	1.3	0.26	4.8	3.5
156	19.7	69.6	10.7	3.8	2.9	1.9	0.47	3.9	2.9
157	90.5	8.9	0.6	9.6	2.8	1.7	0.45	3.7	4.9
1110	1.9	96.1	2.0	1.0	0.9	4.4	0.26	16.8	2.4
1111	14.5	80.0	5.6	3.2	1.7	1.2	0.34	3.6	3.0
1240	3.8	94.8	1.4	1.0	1.5	1.5	0.32	4.5	2.9

ANNEX IX – WEIGHT OF EVIDENCE TO ASSESS SEDIMENT QUALITY IN MANAGEMENT UNITS: APPLICATION TO SADO ESTUARY PORTUGAL: SUPPORT INFORMATION

WEIGHT OF EVIDENCE TO ASSESS SEDIMENT QUALITY IN MANAGEMENT UNITS: APPLICATION TO SADO ESTUARY PORTUGAL

Caeiro, S., Costa, M. H., DelValls, A., Repolho, T., Gonçalves, M., Mosca, A., Coimbra, A. P. and Painho, M. (2004)
Long abstract proceedings of the 4th Workshop Harmonization of impact assessment tools for sediment and dredged materials, SedNet, AZTI and II QAB – CSIC, 10 – 11 June 2004, San Sebastian, Spain, pp. 64 – 68.
(paper in preparation)

Table IX.1 – Toxicity tests results, benthos index and sediment chemistry in 19 management units and available SQG for each contaminant.

	Toxicity*		Benthos				Metals					Sediment parameters				
Manag. Units	Amphipod (% mort)	Urchin (% abnor)	BI bio	Cd (ug/kg)	Pb (ug/kg)	Zn (ug/kg)	Cu (ug/kg)	Cr (ug/kg)	Hg (ug/kg)	As (ug/kg)	SQG-Q metals	% TOM	% FF	% sand	% Gravel	Eh (mV)
HO1	25.75	35.4	3.52	3.90	26.00	149.00	48.00	26.00	0.43	21.00	0.47	6.93	39.40	53.60	9.19	-275.00
HO2	26.75	50.9	4.62	7.00	32.00	242.50	123.50	50.50	0.58	43.50	0.88	5.86	72.02	26.35	1.63	-311.50
HO3	47.50	39.4	4.28	4.15	22.50	164.50	54.00	31.50	0.43	26.00	0.53	11.66	52.95	44.45	2.63	-229.00
HO4	71.25	32.5	2.96	2.30	11.00	74.00	22.00	16.00	0.16	12.00	0.25	4.64	20.84	67.50	11.69	-399.00
HO5	100.00	100.0	4.98	6.40	48.00	295.00	94.00	48.00	0.35	39.00	0.79	10.80	87.09	12.90	0.00	-256.80
HO6	38.75	7.1	4.92	6.20	24.00	221.00	49.00	52.00	0.29	41.00	0.67	9.56	90.51	8.90	0.55	-198.60
LO1	29.75	23.5	2.33	0.60	3.20	8.20	3.50	2.00	0.07	7.00	0.07	0.90	0.62	92.20	7.01	106.25
LO2	82.50	7.4	2.80	0.70	3.00	17.50	3.00	2.50	0.06	7.00	0.08	0.84	1.52	91.30	7.15	47.40
LO3	77.50	18.0	2.63	0.40	3.50	29.00	2.00	1.00	0.06	6.46	0.07	0.72	1.00	96.00	3.04	114.50
MO1	72.50	23.7	2.71	1.05	5.55	33.00	9.00	7.00	0.07	7.55	0.13	2.38	7.87	84.65	6.64	-141.00
MO2	72.50	22.5	2.81	0.80	6.00	47.00	8.00	5.00	0.07	8.00	0.14	2.21	8.17	82.62	7.85	-126.00
MO3	13.75	36.1	2.86	0.95	4.30	16.00	5.50	3.00	0.07	3.65	0.08	1.44	4.52	86.40	9.08	-184.50
MO4	77.50	14.0	2.36	1.00	4.00	34.00	6.00	5.00	0.08	9.00	0.12	1.36	6.60	89.28	4.18	-171.65
MO5	60.00	15.5	2.88	0.80	3.00	22.00	4.00	4.00	0.06	6.00	0.08	2.01	6.59	85.90	7.48	-103.20
MHO1	19.75	16.9	1.00	2.80	24.00	98.00	30.00	20.00	0.19	15.00	0.33	5.74	26.45	59.07	13.40	-189.10
MHO2	58.75	9.4	3.11	2.00	9.40	67.00	24.00	14.00	0.22	13.00	0.23	4.39	27.25	67.40	12.12	-202.00
MHO3	71.25	14.7	2.99	1.55	6.50	65.00	11.50	10.00	0.08	9.50	0.17	3.39	14.15	74.95	3.90	-153.60
MHO4	48.75	14.3	2.99	2.10	8.30	79.00	15.00	15.00	0.07	13.00	0.21	3.83	19.68	69.60	10.69	-210.30
MHO5	86.25	100.0	2.65	2.20	13.00	69.00	15.00	13.00	0.10	11.00	0.22	2.49	11.08	67.95	20.96	74.00
PEL	-	-	-	4.21	112	271	108	160	0.7	41.6	-	-	-	-	-	-
TEL	-	-	-	0.68	30.2	124	18.7	52.3	0.13	7.24	-	-	-	-	-	-

* - HO1, MHO1, sampled at 2/7/03; HO2, LO1, sampled at 3/7/03; HO6; LO2, MO4, MO5, MHO2, MHO4, sampled at 7/10/03; HO3, HO4, HO5, MO3, MHO5, sampled at 2/09/03; LO3, MO1, MO2, MHO3, sampled at 8/10/03.

Table IX.1 – Toxicity tests results, benthos index and sediment chemistry in 19 management units and available SQG for each contaminant (cont.).

Manag. Units	Organochlorine pesticides														
	α-BHC (ug/kg)	γ-BHC (ug/kg) (lindane)	Heptachlor (ug/kg)	δ-BHC (ug/kg)	Aldrin (ug/kg)	Isodrin (ug/kg)	Endossulfan I (ug/kg)	Heptachlor epoxide (ug/kg)	p,p'-DDE (ug/kg)	Dieldrin (ug/kg)	p,p'-DDD (ug/kg)	Endrin (ug/kg)	Endossulfan II (ug/kg)	pp'-DDT (ug/kg)	SQG-Q pest
HO1	0.1 a)	0.59 a)	0.35 a)	18	0.10 a)	0.07 a)	0.22 a)	0.05 a)	0.60 b)	0.10 a)	0.31 a)	0.09 a)	0.60 a)	1.2	0.18
HO2	4.7	0.62 a)	0.37 a)	9.1	0.10 a)	0.07 a)	0.22 a)	0.06 a)	0.62 b)	0.10 a)	0.33 a)	0.09 a)	0.64 a)	1.1	0.19
HO3	0.13a)	0.62 a)	0.37 a)	0.65 a)	0.10 a)	0.07 a)	0.22 a)	0.06 a)	0.62 b)	0.10 a)	1.0 b)	0.09 a)	0.64 a)	0.93	0.20
HO4	0.12 a)	0.62 a)	0.37 a)	2.0	0.11 a)	0.07 a)	0.22 a)	0.06 a)	0.20 a)	0.10 a)	0.34 a)	0.09 a)	0.64 a)	0.09 a)	0.14
HO5	0.14 a)	0.69 a)	4.5	0.54 a)	0.12 a)	0.93	0.26 a)	0.06 a)	2.6	0.11 a)	1.9	1.6	16	2.6	0.30
HO6	0.12 a)	0.56 a)	1.0	7.3	0.10 a)	0.07 a)	0.21 a)	0.22	0.39	0.09 a)	0.31 a)	0.08 a)	0.60 a)	0.48	0.14
LO1	0.12 a)	0.59 a)	0.35 a)	0.54 a)	0.10 a)	0.07 a)	0.21 a)	0.05	0.19 a)	0.10 a)	0.31 a)	0.08 a)	0.60 a)	0.08 a)	0.13
LO2	0.80	1.73 b)	0.35 a)	0.54 a)	0.10 a)	0.07 a)	0.21 a)	1.2	0.20 a)	2.5	0.31 a)	0.09 a)	0.60 a)	0.08 a)	0.48
LO3	0.12 a)	0.56 a)	0.35 a)	3.0	0.10 a)	0.35	0.21 a)	1.1	0.20 a)	0.31	0.31 a)	0.09 a)	0.60 a)	0.08 a)	0.14
MO1	1.5	0.56 a)	0.33 a)	5.6	0.10 a)	0.07 a)	0.21 a)	0.05 a)	0.19 a)	0.09 a)	0.31 a)	0.08 a)	0.60 a)	0.86	0.16
MO2	2.7	0.59 a)	1.1	0.65 a)	0.11 a)	0.07 a)	0.22 a)	0.05 a)	0.20 a)	0.23	0.33 a)	0.09 a)	0.64 a)	0.09 a)	0.14
MO3	0.12 a)	0.57 a)	0.58 a)	0.56 a)	0.10 a)	0.07 a)	0.21 a)	0.05 a)	0.20 a)	0.29 b)	0.31 a)	0.08 a)	1.77 b)	0.1 a)	0.14
MO4	0.62	0.56 a)	0.35 a)	0.54 a)	0.10 a)	0.07 a)	0.21 a)	0.15 b)	0.54	0.22	0.93 b)	0.08 a)	0.60 a)	0.52	0.17
MO5	0.54	0.56 a)	0.35 a)	2.7	0.10 a)	0.07 a)	0.21 a)	0.05 a)	0.58 b)	0.09 a)	0.31 a)	0.08 a)	4.5	0.08 a)	0.13
MHO1	0.13 a)	0.62 a)	0.37 a)	0.65 a)	0.11 a)	0.07 a)	0.23 a)	0.06 a)	0.63	0.24	0.34 a)	0.09 a)	0.64 a)	0.09 a)	0.15
MHO2	0.12 a)	0.62 a)	0.37 a)	0.65 a)	0.11 a)	0.07 a)	0.22 a)	0.06 a)	0.20 a)	0.28	0.99 b)	0.09 a)	0.64 a)	0.86	0.20
MHO3	0.12 a)	0.59 a)	0.35 a)	0.54 a)	0.10 a)	0.07 a)	0.78	0.05 a)	0.60 b)	0.56	0.33 a)	0.09 a)	6.7	1.6	0.22
MHO4	0.12 a)	1.7 b)	0.57 a)	0.55 a)	0.10 a)	0.42	0.21 a)	0.05 a)	0.57 b)	0.35	0.31 a)	0.08 a)	0.58 a)	0.4	0.38
MHO5	0.12 a)	0.56 a)	1.4	1.9	0.10 a)	0.07 a)	0.21 a)	0.05 a)	0.19 a)	0.09 a)	0.93 b)	0.08 a)	0.60 a)	0.51	0.16
PEL	-	0.99	-	-	-	-	-	-	374	4.3	7.81	-	-	4.77	-
TEL	-	0.32	-	-	-	-	-	-	2.07	0.72	1.22	-	-	1.19	-

a) below detection limit.

b) bellow quantification limit.